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AN APPLICATION OF TSCHEBYSCHEFF POLYNOMIALS TO A PROBLEM IN SYMMETRIC FUNCTIONS

By G. S. Mahajani, F.A.Sc.
(*Rajputana University, Jaipur*)
V. R. Thiruvenkatachar
(*Defence Science Organisation, New Delhi*)
AND
V. D. Thawani
(*Gauhati University, Gauhati*)

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1. Introduction

In this note we consider the following *Problem**: Given that the set of variables $(x_1, x_2, \ldots x_n)$ satisfy the conditions:—

(*a*) $0 \leqslant x_1 \leqslant x_2 \leqslant \ldots \leqslant x_n$.

(*b*) The first $n-1$ elementary symmetric functions of the x's have fixed values,

i.e.,

$$\left.\begin{aligned} \Sigma x_1 &= k_1 \\ \Sigma x_1 x_2 &= k_2 \\ &\ldots\ldots\ldots\ldots \\ \Sigma x_1 x_2 \ldots x_{n-1} &= k_{n-1} \end{aligned}\right\} \qquad (1)$$

where $k_1, k_2 \ldots k_{n-1}$ are fixed, but *unspecified*, constants.

(*c*) Maximum and minimum values of successive x's occur alternately, *i.e.*, if x_1 has its minimum value, x_2 has its maximum value, x_3 its minimum value and so on. To find, under the above conditions, the limits of variability of the x's, *i.e.*, to find n numbers $(\alpha_1, \alpha_2, \ldots \alpha_n)$ such that

$$0 \leqslant x_1 \leqslant \alpha_1 \leqslant x_2 \leqslant \alpha_2 \leqslant \ldots \leqslant \alpha_{n-1} \leqslant x_n \leqslant \alpha_n \qquad (2)$$

By the imposition of the condition (*c*) we secure the determination not only of the α's but also of the initially unspecified constants $k_1 \ldots k_{n-1}$.

* This problem was suggested by an example in Goodstein[1] in which, however, there are only two constants k and they are *specified*, viz. $k_1 = 2$, $k_2 = 1$.

According to condition (*c*) we have the following two sets of particular solutions for $(x_1 \ldots . x_n)$:—

	x_1	x_2	x_3	x_4	x_5	. . .
Solution I ..	0	α_2	α_2	α_4	α_4	. . .
Solution II ..	α_1	α_1	α_3	α_3	α_5	. . .

(3)

We shall refer to these two solutions as the two "extreme solutions". The condition (*b*) requires that the elementary symmetric functions of the quantities in the second row shall be equal to the corresponding functions of the third row. We show that, under the above conditions, the problem has a unique solution and that the α's may be determined as the zeros of certain Tschebyscheff polynomials.

In order to orient ourselves on the problem and gain motivation for the solution, we first consider some particular cases: $n = 3, 4, 5, 6$ and then proceed to the general case of any number of variables.

2. Particular Cases

(*a*) $n = 3$, $0 \leqslant x_1 \leqslant \alpha_1 \leqslant x_2 \leqslant \alpha_2 \leqslant x_3 \leqslant \alpha_3$. Here the two extreme solutions for the x's are

$$\left.\begin{matrix} 0, & \alpha_2, & \alpha_2 \\ \alpha_1, & \alpha_1, & \alpha_3 \end{matrix}\right\} \tag{4}$$

The equality of the symmetric functions for the two solutions, imposed by the condition (*b*) of §1 may be expressed by the following identity ("the polynomial identity"):

$$\left.\begin{aligned} \phi(t) &\equiv t(t-\alpha_2)^2 \equiv (t-\alpha_1)^2(t-\alpha_3) + \alpha_1^2\alpha_3 \\ &\equiv t^3 - k_1 t^2 + k_2 t \end{aligned}\right\} \tag{P_3}$$

Equating coefficients of powers of t in (P_3) we get

$$\left.\begin{aligned} 2\alpha_2 &= \alpha_3 + 2\alpha_1 = k_1 \\ \alpha_2^2 &= \alpha_1^2 + 2\alpha_1\alpha_3 = k_2 \end{aligned}\right\} \tag{5}$$

whence we find readily that

$$\alpha_1 : \alpha_2 : \alpha_3 = 1 : 3 : 4 \tag{6}$$

and

$$k_1 : k_2 : \alpha_3 = 6 : 9 : 4.$$

If we take $a_3 = 4$, we have $a_1 = 1$, $a_2 = 3$, $a_3 = 4$. Even in this simplest case it is worth noting that since, according to (P_3),

$$\phi(t) = t(t - a_2)^2$$

$$\phi(t) - a_1{}^2 a_3 = (t - a_1)^2 (t - a_3)$$

$\phi'(t)$ has the roots a_1, a_2, so that we have the identity ("derivative identity")

$$\phi'(t) \equiv 3t^2 - 2k_1 t + k_2 \equiv 3(t - a_1)(t - a_2) \qquad (D_3)$$

This gives

$$\left.\begin{aligned} 3(a_1 + a_2) &= 2k_1 \\ 3a_1 a_2 &= k_2 \end{aligned}\right\} \qquad (7)$$

Combining the k_1-relation in (5) with the k_1-relation in (7) we get at once

$$a_1 : a_2 : a_3 = 1 : 3 : 4$$

as before. The relations (5) give 4 equations for determining the 4 quantities a_1, a_2, k_1, k_2 in terms of a_3, and nothing new is given by (7). Nevertheless it proves convenient in dealing with higher cases to use the relations corresponding to both (5) and (7). Of course, these relations though redundant are mutually consistent.

(*b*) $n = 4$, $0 \leqslant x_1 \leqslant a_1 \leqslant x_2 \leqslant a_2 \leqslant x_3 \leqslant a_3 \leqslant x_4 \leqslant a_4$. The two extreme solutions are here

$$\begin{array}{cccc} 0 & a_2 & a_2 & a_4 \\ a_1 & a_1 & a_3 & a_3 \end{array}$$

and the polynomial identity is

$$\left.\begin{aligned} \phi(t) &\equiv t(t - a_2)^2 (t - a_4) \\ &\equiv (t - a_1)^2 (t - a_3)^2 - a_1{}^2 a_3{}^2 \\ &\equiv t^4 - k_1 t^3 + k_2 t^2 - k_3 t \end{aligned}\right\} \qquad (P_4)$$

Now $\phi'(t)$ has the roots a_1, a_2, a_3 so that the derivative identity is

$$\left.\begin{aligned} \phi'(t) &\equiv 4t^3 - 3k_1 t^2 + 2k_2 t - k_3 \\ &\equiv 4(t - a_1)(t - a_2)(t - a_3) \end{aligned}\right\} \qquad (D_4)$$

Equating coefficients of powers of t in (P_4) and (D_4) we get the following two sets of relations:—

$$\left.\begin{aligned} &2(a_1+a_3)=2a_2+a_4=k_1\\ &2a_1a_3(a_1+a_3)=a_2{}^2a_4=k_3\\ &a_1{}^2+4a_1a_3+a_3{}^2=a_2{}^2+2a_2a_4=k_2\\ &4(a_1+a_2+a_3)=3k_1 \end{aligned}\right\} \quad (8)$$

$$\left.\begin{aligned} &4(a_1a_2+a_2a_3+a_3a_1)=2k_2\\ &4a_1a_2a_3=k_3 \end{aligned}\right\} \quad (9)$$

Combining the k_1-relations in (8) and (9) we get

$$a_1+a_3:a_2:a_4=2:1:2 \quad (10)$$

Again, combination of the k_3-relations in (8) and (9) gives

$$a_1a_3=\tfrac{1}{8}a_4{}^2 \quad (11)$$

Thus a_1, a_3 are the roots of

$$f(x)=x^2-a_4x+\tfrac{1}{8}a_4{}^2=0 \quad (12)$$

and a_2 is the root of $\psi(x)=2x-a_4=0$ (13)

Taking $a_4=4$ we get: $a_1=2-\sqrt{2}$, $a_2=2$, $a_3=2+\sqrt{2}$, $a_4=4$.

(*c*) $n=5$, $0\leqslant x_1\leqslant a_1\leqslant x_2\leqslant a_2\leqslant x_3\leqslant a_3\leqslant x_4\leqslant a_4\leqslant x_5\leqslant a_5$.

The two extreme solutions are now

$$0,\ a_2,\ a_2,\ a_4,\ a_4$$

$$a_1,\ a_1,\ a_3,\ a_3,\ a_5$$

and the polynomial identity becomes

$$\left.\begin{aligned} \phi(t)&\equiv t(t-a_2)^2(t-a_4)^2\\ &\equiv(t-a_1)^2(t-a_3)^2(t-a_5)+a_1{}^2a_3{}^2a_5\\ &\equiv t^5-k_1t^4+k_2t^3-k_3t^2+k_4t \end{aligned}\right\} \quad (P_5)$$

The derivative identity is

$$\left.\begin{aligned} \phi'(t)&\equiv 5t^4-4k_1t^3+3k_2t^2-2k_3t+k_4\\ &\equiv 5(t-a_1)(t-a_2)(t-a_3)(t-a_4) \end{aligned}\right\} \quad (D_5)$$

From these we derive the relations:

$$\left.\begin{aligned} &2(a_2+a_4)=2(a_1+a_3)+a_5=k_1\\ &a_2{}^2+4a_2a_4+a_4{}^2=a_1{}^2+4a_1a_3+a_3{}^2+2a_5(a_1+a_3)=k_2\\ &2a_2a_4(a_2+a_4)=2a_1a_3(a_1+a_3)+a_5(a_1{}^2+a_3{}^2)=k_3\\ &2a_2a_4(a_2+a_4)=2a_1a_3(a_1+a_3)+a_5(a_1{}^2+a_3{}^2)=k_3\\ &a_2{}^2a_4{}^2=a_1{}^2a_3{}^2+2a_1a_3a_5(a_1+a_2)=k_4 \end{aligned}\right\} \quad (14)$$

$$\left.\begin{aligned} 5\Sigma a_1 &= 4k_1 \\ 5\Sigma a_1a_2 &= 3k_2 \\ 5\Sigma a_1a_2a_3 &= 2k_3 \\ 5a_1a_2a_3a_4 &= k \end{aligned}\right\} \tag{15}$$

Here the functions on the l.h.s. are the elementary symmetric functions in (a_1, a_2, a_3, a_4).

Combining the k_1-relations of (14) and (15) we get

$$\left.\begin{aligned} a_1 + a_3 &= \frac{3}{4}a_5 \\ a_2 + a_4 &= \frac{5}{4}a_5 \end{aligned}\right\} \tag{16}$$

while from the k_4-relations we have

$$\left.\begin{aligned} a_1a_3 &= \frac{1}{16}a_5^2 \\ a_2a_4 &= \frac{5}{16}a_5^2 \end{aligned}\right\} \tag{17}$$

Thus a_1, a_3 are the roots of

$$f(x) \equiv x^2 - \frac{3}{4}a_5x + \frac{1}{16}a_5^2 = 0 \tag{18}$$

and a_2, a_4 are the roots of

$$\psi(x) \equiv x^2 - \frac{5}{4}a_5x + \frac{5}{16}a_5^2 = 0 \tag{19}$$

Observe that

$$\frac{5}{2}f(x) = x^{\frac{1}{2}}\frac{d}{dx}\{x^{\frac{1}{2}}\psi(x)\}$$

With $a_5 = 4$, we get:

$$a_1 = \frac{3-\sqrt{5}}{2},\ a_2 = \frac{5-\sqrt{5}}{2},\ a_3 = \frac{3+\sqrt{5}}{2},\ a_4 = \frac{5+\sqrt{5}}{2},\ a_5 = 4$$

(*d*) $n = 6$. With six variables, the polynomial identity is

$$\left.\begin{aligned} \phi(t) &\equiv t(t-a_2)^2(t-a_4)^2(t-a_6) \\ &\equiv (t-a_1)^2(t-a_3)^2(t-a_5)^2 - a_1^2a_3^2a_5^2 \\ &\equiv t^6 - k_1t^5 + k_2t^4 - k_3t^3 + k_4t^2 - k_5t \end{aligned}\right\} \tag{P$_6$}$$

and the derivative identity becomes

$$\left.\begin{aligned}\phi'(t) &\equiv 6t^5 - 5k_1t^4 + 4k_2t^3 - 3k_3t^2 + 2k_4t - k_5 \\ &\equiv 6(t-a_1)(t-a_2)(t-a_3)(t-a_4)(t-a_5)\end{aligned}\right\} \quad (D_6)$$

Equating coefficients of powers of t and combining the k_1-, k_2- and k_5-relations from the two sets so obtained we get

$$\left.\begin{aligned}&\frac{a_1+a_3+a_5}{3} = \frac{a_2+a_4}{2} = \frac{a_6}{2} \\ &\frac{a_1a_3+a_3a_5+a_5a_1}{9} = \frac{a_2a_4}{3} = \frac{a_6^2}{16} \\ &a_1a_3a_5 = \frac{1}{32}a_6^3\end{aligned}\right\} \quad (20)$$

Hence a_1, a_3, a_5 are the roots of

$$f(x) \equiv x^3 - \frac{3}{2}a_6x^2 + \frac{9}{16}a_6^2x - \frac{1}{32}a_6^3 = 0 \quad (21)$$

while a_2, a_4 are the roots of

$$\psi(x) \equiv x^2 - a_6x + \frac{3}{16}a_1^2 = 0 \quad (22)$$

It will be noted that here $\psi(x) = \frac{1}{3}f'(x)$.

With $a_6 = 4$, we thus have

$$a_1 = 2 - \sqrt{3},\ a_2 = 1,\ a_3 = 2,\ a_4 = 3,\ a_5 = 2 + \sqrt{3},\ a_6 = 4.$$

To summarise, we have the following solutions in the particular cases considered above (taking $a_n = 4$ always):

$n = 3$, $(a_1, a_2, a_3) = (1, 3, 4)$

$n = 4$, $(a_1, a_2, a_3, a_4) = (2 - \sqrt{2}, 2, 2 + \sqrt{2}, 4)$

$n = 5$, $(a_1, a_2, a_3, a_4, a_5) = \left(\frac{3-\sqrt{5}}{2}, \frac{5-\sqrt{5}}{2}, \frac{3+\sqrt{5}}{2}, \frac{5+\sqrt{5}}{2}, 4\right)$

$n = 6$, $(a_1, a_2, a_3, a_4, a_5, a_6) = (2 - \sqrt{3}, 1, 2, 3, 2 + \sqrt{3}, 4)$.

It will be observed that for $n = 4$ and $n = 6$, one of the a's has the value $2\,(= \frac{1}{2}a_n)$ and that the remaining a's apart from a_n itself, are symmetrically situated with respect to this.

We shall see that this is true generally for all even values of n. For $n = 3$ and $n = 5$, if we omit a_n, we notice that, of the remaining a's the sum of any pair of quantities equidistant from the two ends is always equal to a_n. This will also be found to be true generally for all odd values of n.

3. General Case of n Variables

In dealing with the general case it is convenient to consider the cases of n odd and n even separately.

Case I.—Odd number of variables, $n = 2m + 1$

$$0 \leqslant x_1 \leqslant a_1 \leqslant x_2 \leqslant a_2 \leqslant \ldots\ldots \leqslant x_{2m} \leqslant a_{2m} \leqslant x_{2m+1} \leqslant a_{2m+1} (= \xi).$$

The two extreme solutions for the x's are

$$\left.\begin{array}{l} 0,\ a_2,\ a_2,\ a_4,\ a_4,\ldots\ldots a_{2m},\ a_{2m} \\ a_1,\ a_1,\ a_3,\ a_3,\ldots\ldots a_{2m-1},\ a_{2m-1},\ \xi \end{array}\right\}$$

We have therefore, on account of the condition (*b*) in § 1, the polynomial identity

$$\left.\begin{array}{l} \phi(t) \equiv t(t-a_2)^2(t-a_4)^2\ldots\ldots(t-a_{2m})^2 \\ \quad \equiv (t-a_1)^2(t-a_3)^2\ldots\ldots(t-a_{2m-1})^2(t-\xi) + \xi a_1{}^2 a_3{}^2 - a^2{}_{2m-1} \\ \quad \equiv t^{2m+1} - k_1 t^{2m} + k_2 t^{2m-1} - \ldots\ldots - k_{2m-1} t^2 + k_{2m} t \end{array}\right\} \quad (\mathrm{P}_{2m+1})$$

For the derivative identity we have

$$\left.\begin{array}{l} \phi'(t) \equiv (2m+1)\, t^{2m} - 2m k_1 t^{2m-1} + (2m-1)\, k_2 t^{2m-2} - \ldots\ldots \\ \qquad\qquad - 2k_{2m-1} t + k_{2m} \\ \quad \equiv (2m+1)(t-a_1)(t-a_2)(t-a_3)\ldots\ldots(t-a_{2m-1})(t-a_{2m}) \end{array}\right\} \quad (\mathrm{D}_{2m+1})$$

Let

$$\left.\begin{array}{l} f(t) \equiv (t-a_1)(t-a_3)\ldots\ldots(t-a_{2m-1}) \equiv t^m - s_1 t^{m-1} + s_2 t^{m-2} - \ldots\ldots \\ \qquad\qquad + (-1)^m s_m \\ \psi(t) \equiv (t-a_2)(t-a_4)\ldots\ldots(t-a_{2m}) \equiv t^m - \sigma_1 t^{m-1} + \sigma_2 t^{m-2} - \ldots\ldots \\ \qquad\qquad + (-1)^m \sigma_m \end{array}\right\} \quad (23)$$

Introducing (23) in (P_{2m+1}) and (D_{2m+1}) we get

$$\left.\begin{array}{l} t[t^m - \sigma_1 t^{m-1} + \sigma_2 t^{m-2} - \ldots\ldots + (-1)^{m-1}\sigma_{m-1} t + (-1)^m \sigma_m]^2 \\ \quad \equiv [t^m - s_1 t^{m-1} + s_2 t^{m-2} - \ldots\ldots + (-1)^{m-1} s_{m-1} t \\ \qquad\qquad + (-1)^m s_m]^2 (t-\xi) + \xi s_m{}^2 \\ \quad \equiv t^{2m+1} - k_1 t^{2m} + k_2 t^{2m-1} - \ldots\ldots - k_{2m-1} t^2 + k_{2m} t \end{array}\right\} \quad (\mathrm{P}'_{2m+1})$$

$$\left.\begin{array}{l} (2m+1)[t^m - \sigma_1 t^{m-1} + \sigma_2 t^{m-2} - \ldots\ldots + (-1)^{m-1}\sigma_{m-1} t + (-1)^m \sigma_m] \\ \quad [t^m - s_1 t^{m-1} + s_2 t^{m-2} - \ldots\ldots + (-1)^{m-1} s_{m-1} t + (-1)^m s_m] \\ \quad \equiv (2m+1)\, t^{2m} - 2m k_1 t^{2m-1} + (2m-1)\, k_2 t^{2m-2} - \ldots\ldots \\ \qquad\qquad - k_{2m-1}\, t + k_{2m} \end{array}\right\} \quad (\mathrm{D}'_{2m+1})$$

Equating coefficients of $t^{2m}, t^{2m-1}, \ldots . t^{m+1}$ in (P'_{2m+1}) and (D'_{2m+1}) we obtain the two sets of relations:

$$\left.\begin{aligned}
&2\sigma_1 = 2s_1 + \xi = k_1 \\
&\sigma_1^2 + 2\sigma_2 = s_1^2 + 2s_2 + 2\xi s_1 = k_2 \\
&2\sigma_3 + 2\sigma_1\sigma_2 = 2s_3 + 2s_1 s_2 = \xi\,(2s_2 + s_1^2) = k_3 \\
&2\sigma_4 + 2\sigma_1\sigma_3 + \sigma_2^2 = 2s_4 + 2s_1 s_3 + s_2^2 + 2\xi\,(s_3 + s_1 s_2) = k_4 \\
&\qquad\qquad \ldots\ldots\ldots\ldots\ldots
\end{aligned}\right\} \quad (24)$$

$$\left.\begin{aligned}
&2\sigma_m + 2\sigma_1\sigma_{m-1} + \ldots . = 2s_m + 2s_1 s_{m-1} + \ldots . + \xi\,(2s_{m-1} \\
&\qquad + 2s_1 s_{m-2} + \ldots .) = k_m \\
&(2m+1)\,(\sigma_1 + s_1) = 2mk_1 \\
&(2m+1)\,(\sigma_2 + \sigma_1 s_1 + s_2) = (2m-1)\,k_2 \\
&(2m+1)\,(\sigma_3 + \sigma_1 s_2 + \sigma_2 s_1 + s_3) = (2m-2)\,k_3 \\
&\qquad\qquad \ldots\ldots\ldots\ldots\ldots
\end{aligned}\right\} \quad (25)$$

$$(2m+1)\,(\sigma_m + \sigma_{m-1}s_1 + \sigma_{m-2}s_2 + \ldots . + \sigma_1 s_{m-1} + s_m) = (m+1)\,k_m.$$

These constitute $3m$ relations for determining the $3m$ quantities $(\alpha_1, \alpha_2, \ldots . \alpha_{2m-1}, \alpha_{2m})$, $(k_1, k_2, \ldots . k_m)$ in terms of ξ*. By combining corresponding relations from (24) and (25) (conveniently labelled by the k's on the r.h.s.), we can solve for the σ_i and s_i in terms of ξ. Thus, by combining the k_1-relations from (24) and (25) we get

$$\frac{\sigma_1}{2m+1} = \frac{s_1}{2m-1} = \tfrac{1}{4}\xi.$$

Next combining the k_2-relations and using the values of σ_1, s_1 we get

$$\frac{\sigma_2}{2m+1} = \frac{s_2}{2m+3} = (m-1)\left(\frac{\xi}{4}\right)^2.$$

Proceeding like this we get the following solution:

$$\frac{\sigma_1}{2m+1} = \frac{s_1}{2m-1} = \frac{\xi}{4}$$

$$\frac{\sigma_2}{2m+1} = \frac{s_2}{2m-3} = (m-1)\left(\frac{\xi}{4}\right)^2$$

$$\frac{\sigma_3}{2m+1} = \frac{s_3}{2m-5} = \frac{1}{3}(m-2)(2m-3)\left(\frac{\xi}{4}\right)^6, \text{ etc.}$$

---

* If we equate the coefficients of *all* powers of t in (P'_{2m+1}) & (D'_{2m+1}) we obtain $3m$ further relations, some of which determine the remaining k's, while the others are identically satisfied in virtue of the rest.

These give

$$\left.\begin{aligned} s_1 &= \binom{2m-1}{1}\left(\frac{\xi}{4}\right) \\ s_2 &= \binom{2m-2}{2}\left(\frac{\xi}{4}\right)^2 \\ &\cdots\cdots\cdots \\ s_m &= \binom{m}{m}\left(\frac{\xi}{4}\right)^m \end{aligned}\right\} \tag{26}$$

and

$$\left.\begin{aligned} \sigma_1 &= \frac{2m+1}{2m-1}\binom{2m-1}{1}\left(\frac{\xi}{4}\right) \\ \sigma_2 &= \frac{2m+1}{2m-3}\binom{2m-2}{2}\left(\frac{\xi}{4}\right)^2 \\ &\cdots\cdots\cdots\cdots\cdots\cdots \\ \sigma_m &= \frac{2m+1}{1}\binom{m}{m}\left(\frac{\xi}{4}\right)^m \end{aligned}\right\} \tag{27}$$

Hence, by (23), $(\alpha_1, \alpha_3, \ldots . \alpha_{2m-1})$ are the roots of

$$f(x) \equiv x^m - \binom{2m-1}{1}\left(\frac{\xi}{4}\right)x^{m-1} + \binom{2m-2}{2}\left(\frac{\xi}{4}\right)^2 x^{m-2} - \ldots .$$
$$+ (-1)^m \binom{m}{m}\left(\frac{\xi}{4}\right)^m = 0 \tag{28}$$

and $(\alpha_2, \alpha_4, \ldots . \alpha_{2m})$ are the roots of

$$\psi(x) \equiv \frac{x^m}{2m+1} - \binom{2m-1}{1}\left(\frac{\xi}{4}\right)\frac{x^{m-1}}{2m-1} + \binom{2m-2}{2}\left(\frac{\xi}{4}\right)^2 \frac{x^{m-2}}{2m-3} - \ldots .$$
$$+ (-1)^m \binom{m}{m}\left(\frac{\xi}{4}\right)^m = 0 \tag{29}$$

If we multiply these equations by $(4/\xi)^m$ and put

$$u = 4x/\xi \tag{30}$$

they become

$$\mathcal{F}(u) \equiv \left(\frac{4}{\xi}\right)^m f\left(\frac{\xi u}{4}\right) \equiv u^m - \binom{2m-1}{1}u^{m-1} + \binom{2m-2}{2}u^{m-2} - \ldots .$$
$$+ (-1)^m \binom{m}{m} = 0 \tag{31}$$

$$\Psi(u) \equiv \left(\frac{4}{\xi}\right)^m \psi\left(\frac{\xi u}{4}\right) \equiv \frac{u^m}{2m+1} - \binom{2m-1}{1}\frac{u^{m-1}}{2m-1} + \binom{2m-2}{2}\frac{u^{m-2}}{2m-3} -$$
$$\ldots . + (-1)^m \binom{m}{m} = 0 \tag{32}$$

Case II.—Even number of variables, $n = 2m$.

$$0 \leqslant x_1 \leqslant a_1 \leqslant x_2 \leqslant a_2 \leqslant \ldots\ldots \leqslant x_{2m-1} \leqslant a_{2m-1} \leqslant x_{2m} \leqslant a_{2m} (= \xi).$$

The polynomial and derivative identities corresponding to (P_{2m+1}) and $(D_{2m,1})$ are now, respectively,

$$\left.\begin{aligned} \phi(t) &\equiv t(t-a_2)^2(t-a_4)^2 \ldots\ldots (t-a_{2m-2})^2 (t-\xi) \\ &\equiv (t-a_1)^2 (t-a_3)^2 \ldots\ldots (t-a_{2m-1})^2 - a_1{}^2 a_3{}^2 \ldots\ldots a^2{}_{2m-1} \\ &\equiv t^{2m} - k_1 t^{2m-1} + k_2 t^{2m-2} - \ldots\ldots + k_{2m-2} t^2 - k_{2m-1} t \end{aligned}\right\} \quad (P_{2m})$$

and

$$\left.\begin{aligned} \phi'(t) &\equiv 2mt^{2m-1} - (2m-1) k_1 t^{2m-2} + (2m-2) k_2 t^{2m-3} - \ldots\ldots \\ &\qquad + 2k_{2m-2} t - k_{2m-1} \\ &\equiv 2m (t-a_1)(t-a_2) \ldots\ldots (t-a_{2m-2})(t-a_{2m-1}) \end{aligned}\right\} \quad (D_{2m})$$

Proceeding as in Case I we now obtain the following results:

$$\left.\begin{aligned} \frac{s_1}{m} &= \frac{\sigma_1}{m-1} = \frac{\xi}{2} \\ \frac{s_2}{m} &= \frac{\sigma_2}{m-2} = (2m-3)\left(\frac{\xi}{4}\right)^2 \\ \frac{s_3}{m} &= \frac{\sigma_3}{m-3} = \tfrac{1}{3}(2m-4)(2m-5)\left(\frac{\xi}{4}\right)^3 \\ &\ldots\ldots\ldots\ldots \\ \frac{s_{m-1}}{m} &= \frac{\sigma_{m-1}}{1} = \binom{m}{m-1}\left(\frac{\xi}{4}\right)^{m-1} \\ s_m &= \frac{2\sigma_{m-1}}{m} \cdot \left(\frac{\xi}{4}\right). \end{aligned}\right\} \quad (33)$$

Thus we find that $(a_2, a_4, \ldots\ldots = a_{2m-2})$ are the roots of

$$\psi_1(x) \equiv x^{m-1} - \binom{2m-2}{1}\left(\frac{\xi}{4}\right) x^{m-2} + \binom{2m-3}{2}\left(\frac{\xi}{4}\right)^2 x^{m-3} - \ldots\ldots$$
$$+ (-1)^{m-2} \binom{m+1}{m-2}\left(\frac{\xi}{4}\right)^{m-2} x + (-1)^{m-1}\binom{m}{m-1}\left(\frac{\xi}{4}\right)^{m-1} = 0 \quad (34)$$

and $(a_1, a_3, \ldots\ldots a_{2m-1})$ are the roots of

$$f_1(x) \equiv \frac{x^m}{m} - \binom{2m-2}{1}\left(\frac{\xi}{4}\right)\frac{x^{m-1}}{m-1} + \binom{2m-3}{2}\left(\frac{\xi}{4}\right)^2 \frac{x^{m-2}}{m-2} \quad (35)$$
$$- \ldots\ldots + (-1)^{m-1}\binom{m}{m-1}\left(\frac{\xi}{4}\right)^{m-1} x + (-1)^m \frac{2}{m}\left(\frac{\xi}{4}\right)^m = 0$$

If as in (30) we write $u = 4x/\xi$, these equations become

$$\Psi_1(u) \equiv \left(\frac{4}{\xi}\right)^{m-1} \psi_1\left(\frac{\xi u}{4}\right) \equiv u^{m-1} - \binom{2m-2}{1} u^{m-2} + \binom{2m-3}{2} u^{m-3}$$

$$- \ldots + (-1)^{m-2} \binom{m+1}{m-2} u + (-1)^{m-1} \binom{m}{m-1} = 0$$

$$\mathcal{F}_1(u) \equiv \left(\frac{4}{\xi}\right)^m f_1\left(\frac{\xi u}{4}\right) \equiv \frac{u^m}{m} - \binom{2m-2}{1} \frac{u^{m-1}}{m-1} + \binom{2m-3}{2} \frac{u^{m-2}}{m-2} - \ldots$$

$$+ (-1)^{m-1} \binom{m}{m-1} u + (-1)^m \frac{2}{m} = 0 \qquad (37)$$

It is to be observed that in Case I, for example,

$$f(x) = 2x^{\frac{1}{2}} \frac{d}{dx} \{x^{\frac{1}{2}} \psi(x)\}$$

so that the roots of $f(x) = 0$ separate those of $\psi(x) = 0$, as indeed they should. A similar remark applies to Case II also, where

$$\psi_1(x) = \frac{d}{dx} f_1(x).$$

The problem is thus reduced to showing that the equations have real roots and to obtaining these roots explicitly if possible. We shall show that both these objects can be attained by reducing the polynomials on the l.h.s. of these equations to Tschebyscheff polynomials.

4. Completion of the Solution by Reduction to Tschebyscheff Polynomials

Consider $\mathcal{F}(u)$. We have

$$\mathcal{F}(u) = \sum_{r=0}^{m} (-1)^r \binom{2m-r}{r} u^{m-r}$$

$$= (-1)^m \sum_{r=0}^{m} (-1)^r \binom{m+r}{m-r} u^r$$

[reversing the order of terms]

$$= (-1)^m \sum_{r=0}^{m} (-1)^r \binom{m+r}{2r} u^r$$

$$= (-1)^m \, \mathrm{F}\left(m+1, \; -m; \; \tfrac{1}{2}; \; \frac{u}{4}\right)$$

in the notation of hypergeometric functions.

Restoring x in place of u, we get

$$f(x) = \left(\frac{\xi}{4}\right)^m \mathcal{F}\left(\frac{4x}{\xi}\right) = (-1)^m \left(\frac{\xi}{4}\right)^m \mathrm{F}\left(m+1, \; -m; \; \tfrac{1}{2}; \; \frac{x}{\xi}\right) \qquad (38)$$

Similarly we find that

$$\psi(x) = \left(\frac{\xi}{4}\right)^m \Psi\left(\frac{4x}{\xi}\right) = (-1)^m \left(\frac{\xi}{4}\right)^m \mathrm{F}\left(m+1,\ -m;\ \frac{3}{2};\ \frac{x}{\xi}\right) \tag{39}$$

$$\psi_1(x) = \left(\frac{\xi}{4}\right)^{m-1} \Psi_1\left(\frac{4x}{\xi}\right) = (-1)^{m-1} \left(\frac{\xi}{4}\right)^{m-1} \mathrm{F}\left(m+1,\ -m+1;\ \frac{3}{2};\ \frac{x}{\xi}\right) \tag{40}$$

$$f_1(x) = \left(\frac{\xi}{4}\right)^m \mathcal{F}_1\left(\frac{4x}{\xi}\right) = (-1)^m \left(\frac{\xi}{4}\right)^m \cdot \frac{2}{m} \mathrm{F}\left(m,\ -m;\ \tfrac{1}{2};\ \frac{x}{\xi}\right) \tag{41}$$

We now make use of the following known results[2]:—

$$\mathrm{F}\left(\frac{1+\mu}{2},\ \frac{1-\mu}{2};\ \tfrac{1}{2};\ x^2\right) = \frac{\cos(\mu \arcsin x)}{(1-x^2)^{\frac{1}{2}}} \tag{42a}$$

$$\mathrm{F}\left(\frac{1+\mu}{2},\ \frac{1-\mu}{2};\ \frac{3}{2};\ x^2\right) = \frac{\sin(\mu \arcsin x)}{\mu x} \tag{42b}$$

$$\mathrm{F}\left(\frac{\mu}{2},\ -\frac{\mu}{2};\ \tfrac{1}{2};\ x^2\right) = \cos(\mu \arcsin x) \tag{42c}$$

$$\mathrm{F}\left(1+\tfrac{1}{2}\mu,\ 1-\tfrac{1}{2}\mu;\ \frac{3}{2};\ x^2\right) = \frac{\sin(\mu \arcsin x)}{\mu x (1-x^2)^{\frac{1}{2}}} \tag{42d}$$

Using these and recalling the definitions of the Tschebyscheff polynomials[3]:

$$\mathrm{T}_n(x) = \cos(n \arccos x)$$

$$\mathrm{U}_n^*(x) = (1-x^2)^{-\frac{1}{2}} \sin\{(n+1) \arccos x\}$$

we find that

$$\left.\begin{aligned}
f(x) &= \left(\frac{\xi}{4}\right)^m \mathrm{U}_{2m}^*\left(\sqrt{x/\xi}\right) = \left(\frac{\xi}{4}\right)^m \frac{\sin\{(2m+1) \arccos \sqrt{x/\xi}\}}{(1-x/\xi)^{\frac{1}{2}}} \\
\psi(x) &= \left(\frac{\xi}{4}\right)^m \cdot \frac{\mathrm{T}_{2m+1}(\sqrt{x/\xi})}{(2m+1)\sqrt{x/\xi}} = \left(\frac{\xi}{4}\right)^m \cdot \frac{\cos(2m+1) \arccos \sqrt{x/\xi}}{(2m+1)\sqrt{x/\xi}} \\
\psi_1(x) &= \left(\frac{\xi}{4}\right)^{m-1} \frac{\mathrm{U}_{2m-1}^*(\sqrt{x/\xi})}{x^{\frac{1}{2}}} = \left(\frac{\xi}{4}\right)^{m-1} \cdot \frac{\sin\{2m \arccos \sqrt{x/\xi}\}}{\sqrt{x}(1-x/\xi)} \\
f_1(x) &= \left(\frac{\xi}{4}\right)^m \cdot \frac{2}{m} \mathrm{T}_{2m}\sqrt{x/\xi} = \frac{2}{m}\left(\frac{\xi}{4}\right)^m \{\cos 2m \arccos \sqrt{x/\xi}\}
\end{aligned}\right\} \tag{43}$$

The above identifications assume that $0 \leqslant x \leqslant \xi$ which, of course, is satisfied since the α's lie in $(0, \xi)$. But it may be mentioned that the reduction of $f(x)$, $\psi(x)$, $f_1(x)$, $\psi_1(x)$ to Tschebyscheff polynomials may be carried out without any restricting condition on x, by starting from the definitions

$$\mathrm{T}_n(x) = \mathrm{F}\left(n,\ -n;\ \tfrac{1}{2};\ \frac{1-x}{2}\right)$$

$$\mathrm{U}_n^*(x) = (n+1)\,\mathrm{F}\left(n+2,\ -n;\ \frac{3}{2};\ \frac{1-x}{2}\right)$$

and using some formulæ of transformation of hypergeometric functions.

It is wellknown that the roots of the polynomials $T_n(x)$, $U_n^*(x)$ are all real and lie in $(-1, +1)$. Therefore the above expressions show that the equations for the α's have all their roots real and located in $(0, \xi)$. Further, these expressions yield the following explicit solutions for the α's in the general case:

(*a*) $n = 2m + 1$:

$$\left.\begin{aligned} \alpha_{2j-1} &= \xi \cos^2 \frac{j\pi}{2m+1} \\ \alpha_{2j} &= \xi \cos^2 \frac{(2j-1)\pi}{2(2m+1)} \end{aligned}\right\} (j = 1, 2 \ldots . m) \qquad (44)$$

$$\alpha_{2m+1} = \xi$$

(*b*) $n = 2m$:

$$\left.\begin{aligned} \alpha_{2j} &= \xi \cos^2 \frac{j\pi}{2m}, \; j = 1, 2, \ldots . (m-1) \\ \alpha_{2j-1} &= \xi \cos^2 \frac{(2j-1)\pi}{4m}, \; j = 1, 2, \ldots . m \end{aligned}\right\} \qquad (45)$$

$$\alpha_{2m} = \xi$$

It is clear that for all even $n\,(= 2m)$, one of the α's has the value ξ. In fact, if $m = 2q$

$$\alpha_{2q} = \tfrac{1}{2}\xi$$

while if $m = 2q - 1$,

$$\alpha_{2q-1} = \tfrac{1}{2}\xi$$

i.e., for all m:

$$\alpha_m = \tfrac{1}{2}\xi.$$

It is also easy to see that, in this case, the remaining α's are symmetrically situated w.r.t. α_m. Further it is easily verified that for odd $n\,(= 2m + 1)$,

$$\alpha_1 + \alpha_{2m} = \alpha_2 + \alpha_{2m-1} = \alpha_3 + \alpha_{2m-2} = \ldots . = \xi.$$

Added in Proof

It will be observed that, if we take the origin at α_0 instead of at O, then for *any* n (odd or even) we have

$$\xi = \alpha_0 + \alpha_n = \alpha_1 + \alpha_{n+1} = \cdots \text{ etc.,}$$
$$= 2\alpha_{n/2} \text{ if } n \text{ is even}$$

Thus there is symmetry from the two ends in all cases.

These properties are illustrated by the particular solutions enumerated in §2.

References

1. Goodstein .. *Mathematical Analysis*, Oxford, 1948, p. 356, Ex. 12.01.
2. Magnus and Oberhettinger .. *Spezielle Functionen d. math. Phys.*, 2nd ed., p. 11.
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SHORTEST SEMIREGULAR CONTINUED FRACTIONS

By M. S. Srinivasan*

(*Research Student, University of Madras*)

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§ 1. *The shortest continued fraction.*—

By a *semiregular continued fraction* (C. F.) of a rational number p/q, we understand a development of the form

$$\frac{p}{q} = a_0 + \frac{\theta_1}{a_1 +} \frac{\theta_2}{a_2 +} \cdots \frac{\theta_r}{a_r}$$

or

$$(a_0\theta_1,\ a_1\theta_2,\ \ldots\ a_{r-1}\theta_r,\ a_r), \tag{1}$$

where a_i's are positive integers,

$$\theta_i = \pm 1;\ a_i \geqslant 1;\ a_r \geqslant 2;\ a_i + \theta_{i+1} \geqslant 1 \quad (0 \leqslant i \leqslant r);$$

in particular, $\theta_1 = +1$ when $a_0 = 0$ and $\theta_{i+1} = +1$ when $a_i = 1$.

Further, if we carry out the division-algorithm in such a way that each remainder

$$\left| \frac{\theta_{i+1}}{(a_{i+1}\ \theta_{i+2},\ \ldots\ a_r)} \right| \leqslant \tfrac{1}{2},$$

we get the † *Nearest Integer Continued Fraction* (N.I.C.F.). Perron has shown that there is a unique N.I.C.F. development for every rational number p/q with the possible exception of the case when the final quotient is 2. For the case $a_r = 2$, there are obviously two developments, since

$$\frac{\theta_{r-1}}{a_{r-1} + 2} \frac{\theta_r}{} = \frac{\theta_{r-1}}{a_{r-1} + \theta_r -} \frac{\theta_r}{2} \qquad (\theta_i = \pm 1).$$

Perron has also remarked that the N.I.C.F. is shortest, in the sense that no other semiregular C.F. of p/q has a smaller number of partial quotients.

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† Perron, *Die Lehre von Kettenbrüchen. Kettenbrüche der nach nächten ganzen*, p. 168.

In fact, there are C.F.'s for some rational numbers p/q, other than the N.I.C.F., which are shortest. For example,

$$\frac{11}{28} = \frac{1}{3-}\ \frac{1}{2+}\ \frac{1}{5} = \frac{1}{2+}\ \frac{1}{2-}\ \frac{1}{6}.$$

I call these *shortest continued fractions.* The nature of these does not seem to have been investigated. In this note I obtain the conditions that a semiregular C.F. may be shortest. I also show how to obtain the number of shortest C.F.'s for p/q in terms of Fibonacci numbers.

Perron shows that the *singular* C.F. for a rational number exists and is unique, but fails to note that it is a case of the shortest C.F. I prove this below and obtain the singular C.F. by a method different from Perron's.

THEOREM 1.—*In the N.I.C.F., the partial quotients* $1+$, $2-$ *do not occur, and conversely.*

Proof.—For, in the N.I.C.F., the partial quotients at each stage is the nearest integer and therefore the remainder

$$\left|\frac{\theta_{i+1}}{(a_{i+1}\ \theta_{i+2}, \ldots . a_r)}\right| \leqslant \tfrac{1}{2}.$$

Hence $a_{i+1} \geqslant 2$; and either $a_{i+1} = 2$, $\theta_{i+2} = +1$, or $a_{i+1} \geqslant 3$. Conversely if these conditions are satisfied, the remainder at each stage is $\leqslant \frac{1}{2}$. When the remainder is $= \frac{1}{2}$ in absolute value, the final stage is reached. Hence the theorem.

§ 2. *Transformation of semiregular C.F.—*

Now, given any semiregular C.F. $(b_0\theta_1,\ b_1\theta_2,\ \ldots .\ b_r)$ for p/q, we proceed to show that it can be transformed into the N.I.C.F. for p/q, *without increasing the number of partial quotients.* (It will follow that the N.I.C.F. for p/q is a shortest C.F. in the sense that no other semiregular C.F. for p/q contains a smaller number of partial quotients).

For this purpose, we have, by Theorem 1 to effect the transformation in such a way that any $1+$ or $2-$ which occur among the partial quotients in

$$(b_0\theta_1,\ b_1\theta_2,\ \ldots .\ b_r) \qquad (2)$$

are removed.

More precisely, we prove that, if (2) contains the partial quotients

$$(a)\ \frac{1}{1+} \quad (b)\ \frac{1}{2-}\frac{1}{2} \quad (c)\ \frac{1}{2-}\frac{1}{2+} \quad (c')\ \frac{1}{2-}\frac{1}{2-}$$

$$(d)\ \frac{1}{2-}\left(\frac{1}{3-}\right)_k^{*}\ \frac{1}{2\pm} \quad (d')\ \frac{1}{2-}\left(\frac{1}{3-}\right)_k\frac{1}{2}$$

$$(e)\ \frac{1}{2-}\frac{1}{a\pm} \quad (a \pm \neq 2 \pm \text{ or } 3-),$$

the $1+$ and $2-$ in these can be transformed away in such a way that there is a reduction in the number of partial quotients in cases (a), (b), (c) (c'), (d), (d') and no reduction in case (e).

Proof.—Firstly, for the case (e), we apply the transformation

$$\frac{1}{\alpha+}\frac{\theta}{2-}\frac{1}{x} = \frac{1}{\alpha+\theta-}\frac{\theta}{2+}\frac{1}{x-1}. \qquad \text{(H)}$$

Consider a C.F. in which this sequence occurs, with the complete quotient $x \geqslant 3$ [so that the sequence comes under (e)] and either $\alpha > 2$; or $\alpha = 2$, $\theta = +1$. The identity (H) shows that the partial quotients can be transformed without reducing the length, so that $2-$ is replaced by $2+$ and no new $2-$ is introduced. This transforms (e) at every stage where (e) occurs, without reducing the length.

Next for reducing (a), (b), (c), (c'), (d), (d') respectively, the following transformations, each of which reduces the number of partial quotients by one [except (c') where the length is reduced by k] are applied:—

$$(a)\ a_i + \frac{\theta_{i+1}}{1+}\frac{1}{a_{i+2}+x} = (a_i+\theta_{i+1}) - \frac{\theta_{i+1}}{a_{i+2}+x+1};$$

$$(b)\ x + \frac{\theta}{2-}\frac{1}{2} = (x+\theta) - \frac{\theta}{3};$$

$$(c)\quad \frac{1}{a+}\frac{\theta}{2-}\frac{1}{2+}\frac{1}{x} = \frac{1}{a+\theta-}\frac{\theta}{2+}\frac{1}{1+}\frac{1}{x} \text{ by (H)}$$

$$= \frac{1}{a+\theta-}\frac{\theta}{3-}\frac{1}{x+1} \text{ by } (a).$$

$$(c')\ \frac{1}{a+}\frac{\theta}{2-}\left(\frac{1}{2-}\right)_K\frac{1}{x} = \frac{1}{a+}\frac{\theta}{2-}\left(\frac{1}{2-}\right)_{K-2}\frac{1}{2-}\frac{1}{2-}\frac{1}{x}$$

$$\text{which by (H)} = \frac{1}{a+}\frac{\theta}{2-}\left(\frac{1}{2-}\right)_{k-2}\frac{1}{1+}\frac{1}{2+}\frac{1}{x-1}$$

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* $\frac{1}{a+}\frac{1}{3-}\frac{1}{3-}\frac{1}{3-}\frac{1}{3-}\frac{1}{b}$ is written as $\frac{1}{a+}\left(\frac{1}{3-}\right)_4\frac{1}{b}$.

which by $(a) = \dfrac{1}{a+}\dfrac{\theta}{2-}\left(\dfrac{1}{2-}\right)_{k-3}\dfrac{1}{1+}\dfrac{1}{3+}\dfrac{1}{x-1}$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

$$= \frac{1}{a+}\frac{\theta}{2-}\left(\frac{1}{2-}\right)_0\frac{1}{1+}\frac{1}{k+}\frac{1}{x-1}$$

$$= \frac{1}{a+}\frac{\theta}{2-}\frac{1}{1+}\frac{1}{k+}\frac{1}{x-1}$$

$$= \frac{1}{a+}\frac{\theta}{1+}\frac{1}{k+1+}\frac{1}{x-1}$$

$$= \frac{1}{a+\theta-}\frac{\theta}{k+2+}\frac{1}{x-1}.$$

(*d*) $\dfrac{1}{a+}\dfrac{\theta}{2-}\left(\dfrac{1}{3-}\right)_k\dfrac{1}{2\pm}\dfrac{1}{x} = \dfrac{1}{a+}\dfrac{\theta}{2-}\dfrac{1}{3-}\left(\dfrac{1}{3-}\right)_{k-1}\dfrac{1}{2\pm}\dfrac{1}{x}$

which by (H) $= \dfrac{1}{a+\theta-}\dfrac{\theta}{2+}\dfrac{1}{2-}\dfrac{1}{3-}\left(\dfrac{1}{3-}\right)_{k-2}\dfrac{1}{2\pm}\dfrac{1}{x}$

$$= \frac{1}{a+\theta-}\frac{\theta}{3-}\frac{1}{2+}\frac{1}{2-}\left(\frac{1}{3-}\right)_{k-2}\frac{1}{2\pm}\frac{1}{x}$$

$$= \frac{1}{a+\theta-}\frac{\theta}{3-}\left(\frac{1}{3-}\right)_1\frac{1}{2+}\frac{1}{2-}\left(\frac{1}{3-}\right)_{k-3}\frac{1}{2\pm}\frac{1}{x}$$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

$$= \frac{1}{a+\theta-}\frac{\theta}{3-}\left(\frac{1}{3-}\right)_{k-2}\frac{1}{2+}\frac{1}{2-}\frac{1}{2\pm}\frac{1}{x}$$

$$= \frac{1}{a+\theta-}\frac{\theta}{3-}\left(\frac{1}{3-}\right)_{k-1}\frac{1}{2+}\frac{1}{1\pm}\frac{1}{x}$$

But $$\frac{1}{2+}\frac{1}{1+}\frac{1}{x} = \frac{1}{3-}\frac{1}{x+1}$$

and $$\frac{1}{2+}\frac{1}{1-}\frac{1}{x} = \frac{1}{3+}\frac{1}{x-1}$$

Hence we have,

$$\frac{1}{a+}\frac{\theta}{2-}\left(\frac{1}{3-}\right)_k\frac{1}{2+}\frac{1}{x} = \frac{1}{a+\theta-}\frac{\theta}{3-}\left(\frac{1}{3-}\right)_{k-1}\frac{1}{3-}\frac{1}{x+1}$$

$$\frac{1}{a+}\frac{\theta}{2-}\left(\frac{1}{3-}\right)_k\frac{1}{2-}\frac{1}{x} = \frac{1}{a+\theta-}\frac{\theta}{3-}\left(\frac{1}{3-}\right)_{k-1}\frac{1}{3+}\frac{1}{x-1}$$

(d') Similarly,

$$\frac{1}{a+}\,\frac{\theta}{2-}\left(\frac{1}{3-}\right)_k\,\frac{1}{2} = \frac{1}{a+\theta-}\,\frac{\theta}{3-}\left(\frac{1}{3-}\right)_{k-2}\,\frac{1}{2+}\,\frac{1}{2-}\,\frac{1}{2}$$

$$= \frac{1}{a+\theta-}\,\frac{\theta}{3-}\left(\frac{1}{3-}\right)_{k-1}\,\frac{1}{3}.$$

This proves all our assertions.

Hence it incidentally follows that the shortest C.F.'s are precisely those which

(1) do not contain the partial quotient $1+$, and

(2) which contain the partial quotient $2-$, if at all, in a manner different from (b), (c), (c'), (d) and (d').

This specifies the shortest C.F.'s completely.

§ 3. *The number of shortest C.F.'s for p/q.*—

This number can be stated in terms of the N.I.C.F. for p/q rendered unique, if necessary, by taking the last partial remainder in the form $+\frac{1}{2}$.

The above proof shows that wherever the partial quotient $\frac{\theta}{2+}$ occurs in the N.I.C.F., then by (H) it can be transformed into $2-$ without increasing the number of partial quotients. This transformation will however introduce another $2+$ in the case when $a=3$, $\theta=-1$ which could be transformed again by (H).

Thus the places in the N.I.C.F. which can be transformed into shortest C.F.'s are those where there are sequences of the form

$$S = \frac{1}{a\pm}\left(\frac{1}{3-}\right)_{a_1}\left(\frac{1}{2+}\right)_{b_1}\left(\frac{1}{3-}\right)_{a_2}\cdots\cdots\left(\frac{1}{2+}\right)_{b_t}\frac{1}{p\pm},$$

which may be more conveniently written as

$$S = a\pm\,(\bar{3})_{a_1}\,(2)_{b_1}\,(\bar{3})_{a_2}\cdots\cdots\,(2)_{b_t}\,p^{\pm},$$

where $a\pm \neq 2+$ or $3-$; $a_i,\ b_i \geqslant 0$; $p>2$.

Let the number of shortest C.F. equivalents to this sequence S be $C(a_1, b_1, a_2, \ldots a_b, b_t)$. If there are several sequences, of the form S in the N.I.C.F., the total number of equivalent shortest C.F.'s is evidently the product of the numbers $C(a_1, b_1, \ldots b_t)$ associated with each of the sequences.

It will be seen from what follows that this number is not affected even if the N.I.C.F. ends with the sequence; *i.e.*, even if p does not exist.

We proceed to obtain a reduction formula to calculate the number of shortest C.F. equivalents to S.

§4. *Reduction formula.—*

THEOREM 2.—*The number of shortest C.F. equivalents to S satisfies the reduction formula*

$$C(a_1, b_1, a_2, \ldots . b_t) =$$

$$\begin{cases} C(0, b_1 - 1, a_2, \ldots . b_t) + (a_1 + 1).C(0, b_1 - 2, a_2 \ldots . b_t) \text{ if } b_1 > 1. \\ C(a_2, b_2, \ldots . b_t) + (a_1 + 1).C(a_2 - 1, b_2, \ldots . b_t) \text{ if } b_1 = 1. \end{cases}$$

Proof.—We divide the shortest C.F. equivalents to S into classes $\Gamma_i (i = 0; 1, 2, \ldots . a_1 + 1)$ respectively, given by:—

(i) Γ_0 = the class of equivalents beginning with α not followed by $\bar{3}$; *i.e.*, of the form

(*a*) $\alpha\, 2\, \bar{2}\, (3)_{a_1 - 1} 3$ followed by M = the transformations of $(2)_{b_1 - 2}\, (3)_{a_2} \ldots . p$, when $b_1 > 1$;

or (*b*) $\alpha\, 2\, \bar{2}\, (\bar{3})_{a_1 - 1}\, \bar{4}$ followed by N = the transformations of

$(\bar{3})_{a_2 - 1}\, (2)\, b_2 \ldots . p$ when $b_1 = 1$.

(ii) Γ_i $(i = 1, 2, \ldots . a_1 - 1)$ = the class of equivalents beginning with $\alpha\, (3)_i$ not followed by $\bar{3}$; *i.e.*, of the form

(*a*) $\alpha\, (3)_i\, 2\, \bar{2}\, (\bar{3})_{a_1 - i - 1} 3$ followed by M when $b_1 > 1$,

or (*b*) $\alpha\, (\bar{3})_i\, 2\, \bar{2}\, (\bar{3})_{a_1 - i - 1}\, \bar{4}$ followed by N when $b_1 = 1$.

(iii) Γ_{a_1} = the class of equivalents beginning with $\alpha\, (\bar{3})_{a_1}$ not followed by 3; *i.e.*, of the form

(*a*) $\alpha\, (\bar{3})_{a_1}\, 2$ followed by transformations of $(2)_{b_1 - 2}\, (3)_{a_2}\, (2)_{b_2} \ldots . p$ when $b_1 > 1$,

or (*b*) $\alpha\, (\bar{3})_{a_1} 2$ followed by transformations of $(3)_{a_2}\, (2)_{b_2} \ldots . p$ when $b_1 = 1$.

(iv) $\Gamma_{a_1 + 1}$ = the class of equivalents not beginning with α; *i.e.*, of the form

(*a*) $\overline{(\alpha + 1)}\, 2\, (\bar{3})_{a_1} 3$ followed by M when $b_1 > 1$

or (*b*) $\overline{(\alpha + 1)}\, 2\, (\bar{3})_{a_1}\, \bar{4}$ followed by N when $b_1 = 1$.

We obtain the forms stated above by application of (H) to the class Γ_{a_1} with $a = 2$, $\theta = 1$ in succession, by which $\bar{3}\,2\,2$ becomes $2\bar{2}3$ and $\bar{3}\,2\,\bar{2}$ becomes $2\,2\bar{3}$. H shows that if the first 2 in $(3)_{a_1}\,(2)_{b_1}$ is transformed by (H), the preceding $\bar{3}$ will be changed.

The number of shortest C.F. equivalents in Γ_{a_1} is $C(o, b_1 - 1, a_2, \ldots . b_t)$ when $b_1 > 1$, and $C(a_2, b_2, \ldots . b_t)$ when $b_1 = 1$.

The number of shortest C.F. equivalents in *each* of the other classes is

$$= C(0, b_1 - 2, a_2, \ldots . b_t) \text{ when } b_1 > 1 \text{ and}$$
$$= C(a_2 - 1, b_2, \ldots . b_t) \text{ when } b_1 = 1.$$

Hence the total number of shortest C.F. equivalents in S is

$$C(0, b_1 - 1, a_2, \ldots . b_t) + (a_1 + 1).C(o, b_1 - 2, a_2, \ldots . b_t) \text{ when } b_1 > 1$$

and

$$C(a_2, b_2, \ldots . b_t) + (a_1 + 1)\, C(a_2 - 1, b_2, \ldots . b_t) \text{ when } b_1 = 1.$$

Corollary.—The shortest C.F. in which $2^{\pm}$ is not preceded by k occurs *only in* the class Γ_0 when a^{+} is the first quotient in S. If $\bar{a}$ is the first quotient, the shortest C.F. of the above type occurs *only in* the class Γ_{a_1+1}. (This will be used to prove the uniqueness of the singular C.F., in Theorem 3.)

By successive application of the reduction formula, the evaluation of $C(a_1, b_1, \ldots . b_t)$ is obtained finally in terms of $C(\alpha, \beta)$. Now we find $C(\alpha, \beta)$ explicitly in terms of Fibonacci numbers.

We have,

$$C(\alpha, \beta) = C(0, \beta - 1) + (\alpha + 1).C(0, \beta - 2)$$

and $$C(0, \beta) = C(0, \beta - 1) + C(o, \beta - 2).$$

Now $C(0, 0)$ = the number of shortest C.F.'s in $\dfrac{1}{\alpha + \dfrac{1}{p}}$ when $\alpha > 2$, $p > 2$, which $= 1$. Also $C(0, 1)$ = the number of shortest C.F.'s in $\dfrac{1}{\alpha + 2 + \dfrac{1}{p}}$ by definition, which $= 2$; these two being evidently given by:

$$\frac{1}{\alpha \pm 2 + \dfrac{1}{p}} = \frac{1}{\alpha \pm 1 \mp 2 - \dfrac{1}{p + 1}}.$$

Now write

$$C(0, \beta) = f(\beta + 1) \text{ so that}$$

$$f(1) = 1;\ f(2) = 2;\ \text{and } f(\beta + 1) = f(\beta) + f(\beta - 1).$$

Hence,

$$f(3) = 3,\ f(4) = 5,\ f(5) = 8, \ldots . f(0) = 1,$$
$$f(-1) = 0,\ f(-2) = 1,\ f(-3) = -1 \ldots .$$

are the Fibonacci numbers. Thus, the C-function may be considered as a generalisation of Fibonacci numbers.

We see that

$$C(a_1, a_2, \ldots . a_{i-1}, 0, a_{i+1}, \ldots . a_{2n}) =$$
$$C(a_1, a_2, \ldots ., a_{i-1} + a_{i+1}, \ldots . a_{2n}).$$

As a particular case $C(2, 3) = 9$; this may be verified by writing down explicitly the nine shortest C.F.'s for $\frac{106}{277}$ whose N.I.C.F. is

$$0 + \frac{1}{3-}\frac{1}{3-}\frac{1}{2+}\frac{1}{2+}\frac{1}{2+}\frac{1}{3}$$

The nine shortest C.F.'s are:—

(i) $0 + \frac{1}{3-}\frac{1}{3-}\frac{1}{2+}\frac{1}{2+}\frac{1}{2+}\frac{1}{3}$

(ii) $0 + \frac{1}{2+}\frac{1}{2-}\frac{1}{3-}\frac{1}{3+}\frac{1}{2+}\frac{1}{3}$

(iii) $0 + \frac{1}{3-}\frac{1}{2+}\frac{1}{2-}\frac{1}{4-}\frac{1}{2-}\frac{1}{4}$

(iv) $0 + \frac{1}{3-}\frac{1}{2+}\frac{1}{2-}\frac{1}{3+}\frac{1}{2+}\frac{1}{3}$

(v) $0 + \frac{1}{2+}\frac{1}{2-}\frac{1}{3-}\frac{1}{4-}\frac{1}{2-}\frac{1}{4}$

(vi) $0 + \frac{1}{3-}\frac{1}{3-}\frac{1}{3-}\frac{1}{2-}\frac{1}{3+}\frac{1}{3}$

(vii) $0 + \frac{1}{3-}\frac{1}{3-}\frac{1}{2+}\frac{1}{3-}\frac{1}{2-}\frac{1}{4}$

(viii) $1 - \frac{1}{2-}\frac{1}{3-}\frac{1}{3-}\frac{1}{3+}\frac{1}{2+}\frac{1}{3}$

(ix) $1 - \frac{1}{2-}\frac{1}{3-}\frac{1}{3-}\frac{1}{4-}\frac{1}{2-}\frac{1}{4}$.

§5. *Singular continued fractions.*—

A semi-regular C.F.

$$a_0 + \frac{\theta_1}{a_1+}\frac{\theta_2}{a_2+} \ldots . \frac{\theta_r}{a_r}$$

is said to be *singular* if

$$a_i \geqslant 2; \quad (a_i + \theta_i) \geqslant 2; \quad \theta_i = \pm 1 \ (0 \leqslant i \leqslant r).$$

This implies that $1 \pm$ and $\frac{-1}{2 \pm}$ do not occur as partial quotients. Hence no sequence of forms (*a*), (*b*), (*c*), (*c'*), (*d*), (*d'*) occurs. Therefore by our previous remark, the singular C.F. is a shortest C.F.

THEOREM 3.—*The singular C.F. for p/q exists and is unique.*

Proof.—By examining the classes Γ_0, Γ_i, Γ_{a_1}, and Γ_{a_1+1} of shortest C.F. equivalents to S, we see that the condition for singularity can be satisfied *only in* the class Γ_0 or Γ_{a_1+1} according as α or $\bar{\alpha}$ is the first quotient in S. (Theorem 2 corollary). The next sequence (of the form S) in this class contains the singular C.F. in the corresponding Γ_0 or Γ_{a_1+1} class of that sequence. Proceeding in this manner, with every successive sequence, we will see finally that the singular C.F. for p/q exists, and is unique.

The singular C.F. can be written down, given the sequence S, applying the following results:—

(1) If $S = \alpha\,(2)_n\,p$ then S.C.F. $= \alpha\,(2)_n\,p$,

(2) If $S = \alpha\,(\bar{3})_m\,(2)_n\,p$ then S.C.F. $= \alpha 2\bar{2}\,(\bar{3})_{m-1}\,3\,(2)_{n-2}p$,

(3) If $S = \bar{\alpha}\,(2)_n\,p$ then S.C.F. $= (\alpha - 1)\,\bar{2}3\,(2)_{n-2}p$,

(4) If $S = \bar{\alpha}\,(\bar{3})_m\,(2)_n\,p$ then S.C.F. $= (\alpha - 1)\,\bar{2}\,(\bar{3})_m\,3\,(2)_{n-2}\,p$,

(5) If $S = \alpha\,(\bar{3})_m\,2p$ then S.C.F. $= \alpha\,2\,\bar{2}\,(\bar{3})_{m-1}\,(p+1)$,

(6) If $S = \bar{\alpha}\,(\bar{3})_m\,2p$ then S.C.F. $= (\alpha - 1)\,\bar{2}\,(\bar{3})_m\,(p+1)$.

Another method for obtaining the S.C.F. (Singular C.F.) is by direct transformation of the N.I.C.F. of p/q. In the N.I.C.F. $2 -$ does not occur. We transform $\frac{-1}{2+}$ into $\frac{+1}{2-}$ by (H), wherever the former occurs in the N.I.C.F. The C.F. finally obtained contains same number of partial quotients as the N.I.C.F. and satisfies the conditions for singularity. This is the singular C.F. of p/q.

If the N.I.C.F. does not contain $\frac{-1}{2+}$, it is itself the singular C.F. If the last term of the N.I.C.F. is $-\frac{1}{2}$, it is transformed to $\frac{+1}{2-}$; for, the singular C.F. does not contain $\frac{-1}{2-}$ as last term.

A NEW SYNTHESIS OF MENAPHTHONE AND LAWSONE

By A. C. Jain and T. R. Seshadri, F.A.Sc.

(From the Department of Chemistry, University of Delhi)

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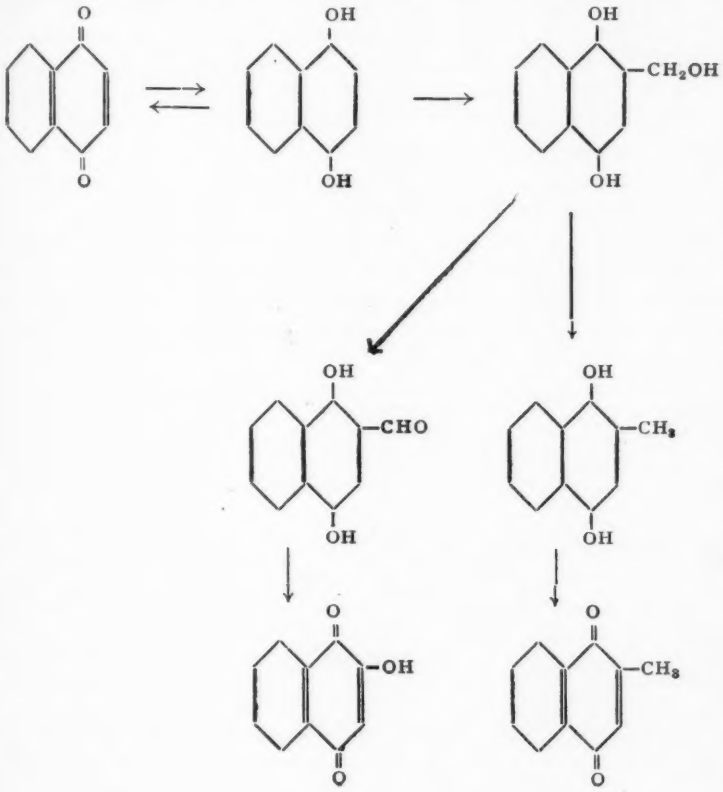
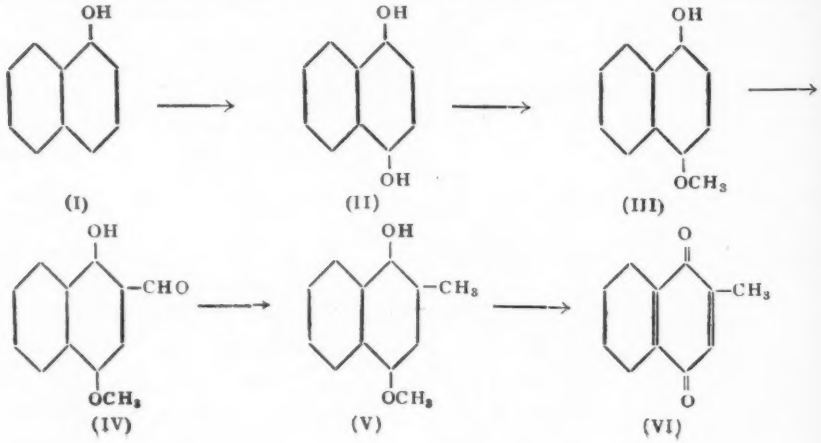
The naphthoquinone nucleus has been found to occur in a large number of natural products. In most of these compounds, there is present in the 2-position a methyl or a hydroxyl group. In the analogous case of anthraquinones, the 2-position frequently contains besides these two substituents a carbinol or a carboxyl group. Probably these are related and all these



groups have a common origin. They may arise by the condensation of formaldehyde or its biological equivalent in the 2-position and subsequent transformation. This point has already been discussed in connection with the nuclear oxidation of flavones.[1] The above biogenetic scheme may be suggested for the naphthoquinone derivatives.

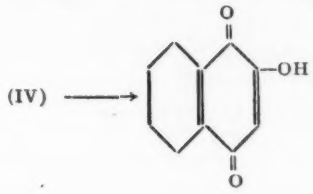
The applicability of the above scheme has now been in the first instance examined using menaphthone (VI) and lawsone (VII) as appropriate examples. For the former, the synthesis starts with α-naphthol (I). It is converted into 1 : 4-dihydroxy naphthalene (II) by oxidation using alkaline persulphate. This substance was prepared earlier by oxidation with chromic acid of naphthalene, α-naphthylamine, α-naphthol, 1 : 4-diamino-naphthalene or 1-hydroxy-4-amino-naphthalene[2] and subsequent reduction of the resulting α-naphthoquinone with sulphur dioxide, stannous chloride and hydrochloric acid or sodium hydrosulphite.[3] More recently Desai and Sethna[4] prepared it from α-naphthol by Elb's persulphate oxidation using potassium persulphate. Their yield of 22% could now be raised to 40% by using the more readily soluble ammonium persulphate. The quinol condenses with hexamine giving very poor yield (1%) of the corresponding 2-aldehyde. Gatterman's method using hydrocyanic acid is better (yield 10%) but not good enough. On the other hand, if the monomethyl ether of quinol (III) which is conveniently prepared by partial methylation employing methyl alcoholic hydrogenchloride,[5] is used for the hexamine condensation, a satisfactory yield (50%) of the 2-aldehyde (IV) is obtained. This undergoes smooth reduction by Clemmensen method yielding 1-hydroxy-4-methoxy-2-methyl-naphthalene (V). Subsequent oxidative-demethylation[6] using nitric acid



produces menaphthone (VI) in a good yield. The stages in this synthesis are represented by the above formulæ.

The above scheme offers a convenient route for obtaining this valuable synthetic vitamin which is in large use. The common method used so far for its preparation is based on the oxidation of 2-methyl naphthalene employing either chromic acid,[7] hydrogen peroxide or molecular oxygen.[8] The yield is claimed to be somewhere within 40–50%. This hydrocarbon is found as a component of low temperature coal tar and its availability would appear to be somewhat limited. Several methods have therefore been examined for its synthesis. (*a*) Reduction of β-naphthaldehyde[9] obtained from β-naphthonitrile which in its turn is prepared from β-naphthylamine or naphthalene-β-sulphonic acid. (*b*) Friedel and Craft's reaction using tetralin, methyl bromide and aluminium bromide and subsequent dehydrogenation with sulphur.[10] But all these methods involve so many steps giving poor yields that accessibility to synthetic 2-methyl naphthalene has been rather difficult.

Lawsone (VII) is 2-hydroxy-α-naphthoquinone and it occurs in the leaves of *Lawsonia alba* and *Lawsonia inermis* and has been synthesised earlier by methods having a large number of steps. The most important method that gives a good yield is that of Fieser[11] which involves six steps starting from β-naphthol. It has now been prepared by the oxidation of 1-hydroxy-4-methoxy-2-naphthaldehyde with alkaline hydrogen peroxide.

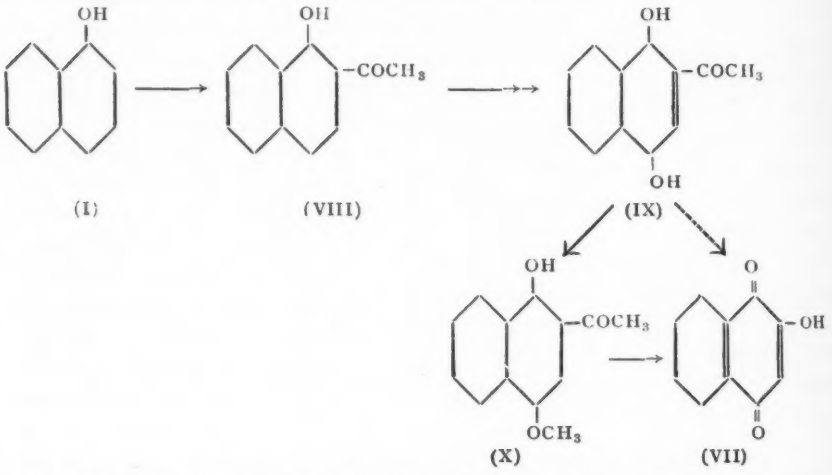


(VII)

In the above Dakin's reaction not only is the 2-aldehydic group substituted by a hydroxyl group, but there is further oxidative demethylation giving rise to the quinone structure. This type of oxidative demethylation in alkaline medium is rather unusual but one case was earlier observed in connection with alkali fission of gardenin where atmospheric oxygen seems to be the oxidising agent.[12]

A modification of the above biogenetic procedure has also been explored starting again with α-naphthol. The 2-acetyl derivative (VIII) is prepared by Nencki's method (Witt and Braun[13]). It undergoes persulphate oxida-

tion yielding 2-acetyl-α-naphthohydroquinone[4] (IX). Subsequent oxidation with hydrogen peroxide produces lawsone (VII).



This appears to be a convenient laboratory method for the preparation of lawsone as the stages are few in number and easy and the yield is satisfactory.

In order to provide a further example of the oxidative demethylation observed in the case of 1-hydroxy-4-methoxy-2-naphthaldehyde (IV) in alkaline hydrogen peroxide, the corresponding ketone, 1-hydroxy-4-methoxy-2-acetyl naphthalene (X) has been prepared by partial methylation of 1:4-dihydroxy-2-acetyl naphthalene using dimethyl sulphate and oxidised with alkaline hydrogen peroxide. Lawsone is obtained directly as expected. Hence it could be concluded that this reaction is of a general nature.

EXPERIMENTAL

1-Hydroxy-4-methoxy-2-naphthaldehyde (IV)

α-Naphthohydroquinone (II) was prepared by the reduction of α-naphthoquinone with sodium hydrosulphite[3] as well as by the persulphate oxidation of α-naphthol.[4] In the latter method it was observed that the use of good ammonium persulphate instead of potassium persulphate increased the yield to 40–45%.

The above quinol was partially methylated according to the method of D.R.P. 173730 with a small modification suited to laboratory conditions. 1:4-Dihydroxy-naphthalene was dissolved in the minimum amount of cold dry 10% methyl alcoholic hydrogen chloride and the solution thus obtained

was left at ordinary temperature for 6–7 hours. The solution was diluted when the monomethyl ether (III) separated in a crystalline condition. It was filtered, washed with a little dilute methyl alcohol and dried (yield, 90%). It crystallised from benzene or petroleum-ether in small colourless needles melting at 130–31°. With alcoholic ferric chloride it gives a beautiful deep blue solution which on keeping separates as a blue precipitate. With concentrated sulphuric acid it gives violet red colour.

An aldehyde group was introduced in the 2-position of the above quinol monomethyl ether by the hexamine and Gatterman methods.

(*a*) *Hexamine method.*—1-Hydroxy-4-methoxy naphthalene (5 g.) was dissolved in dry glacial acetic acid (150 c.c.) and to it hexamine (15 g.) was added. The whole mixture was refluxed on a boiling water-bath under dry conditions. After six hours, boiling dilute hydrochloric acid (1 : 1, 80 c.c.) was added to it and the solution so obtained was heated on a boiling water-bath for 10 minutes. It was left overnight in the refrigerator, when pale yellow needles of 1-hydroxy-4-methoxy-2-naphthaldehyde separated out. It was filtered, washed with water and crystallised from ligroin when it came out as golden yellow tiny needles (2·5 g.) melting at 100–1°. More of the aldehyde (0·5 g.) could be obtained from the mother-liquor by salting out, extraction with ether, washing the ethereal layer first with 10% sodium bicarbonate solution and then with water. The ethereal layer was separated, dried over sodium sulphate and then the ether removed. The residue was dissolved in the least quantity of alcohol; addition of water drop by drop first precipitated out impurities and then the aldehyde as greenish yellow mass which on crystallisation from petroleum ether gave pure aldehyde. (Total yield, 3 g.)

The aldehyde is soluble in alcohol and petroleum ether, moderately soluble in benzene and insoluble in water. It dyes skin an intense yellow and dissolves in alkalies to give a deep yellow solution. With alcoholic ferric chloride it gives a dark green colour. All these tests agree with those recorded for 1-hydroxy-4-methoxy-2-naphthaldehyde by Friedlander[14] who obtained it by alkaline degradation of methoxy-naphthalene-indole-indigo.

(*b*) *Gatterman's method.*—Dry 1-hydroxy-4-methoxy naphthalene (10 g.) and freshly fused zinc chloride (10 g.) were dissolved in anhydrous ether (200 c.c.) and dry hydrogen cyanide (10 c.c.) was added. A rapid stream of dry hydrogen chloride gas was passed into this solution (cooled to 0°) during a period of 3–4 hours, when a yellow oily liquid separated at the bottom. After keeping it overnight in ice-chest, ether was decanted off carefully; the oily liquid was washed with dry ether, and heated with water

(150 c.c.) to boiling for fifteen minutes. The insoluble residual liquid was separated by decanting off the aqueous layer completely. The former solidified on cooling in ice-salt mixture and on stirring with a little amount of alcohol gave a yellow crystalline solid (2·5 g.). This crystallised from petroleum ether as tiny yellow needles melting at 98–99°. The aqueous solution also on cooling yielded more of the aldehyde (0·5 g.).

1-*Hydroxy*-4-*methoxy*-2-*methyl naphthalene* (V)

Powdered granulated zinc (10 g.) was taken in a 250 c.c. round-bottomed flask and shaken with a mixture of water (15 c.c.), concentrated hydrochloric acid (0·5 c.c.) and mercuric chloride (1 g.) for ten minutes. The supernatant solution was then decanted off and the amalgamated zinc thus obtained was covered with a mixture of water (10 c.c.) and conc. hydrochloric acid (10 c.c.). 1-Hydroxy-4-methoxy-2-naphthaldehyde (1 g.) dissolved in alcohol or glacial acetic acid (15 c.c.) was added to it and the whole mixture refluxed in a boiling water-bath for eight hours. During this period conc. hydrochloric acid (4 c.c.) was added after every one hour. The solution was decanted off and diluted with water and left in the refrigerator overnight, when tiny needles (0·4 g.) separated out. It crystallised from petroleum ether as colourless flat needles and narrow rectangular plates melting at 100–2°. More of the reduction product (0·15 g.) could be obtained by extracting with ether the zinc residues as well as the mother-liquor after salting it out. The extract, after being dried over anhydrous sodium sulphate, was treated with animal charcoal and filtered through a fluted filter-paper. Ether was completely removed and the residue was extracted with petroleum ether. The latter on concentration and cooling gave colourless, tiny needles (Found: C, 76·2; H, 6·4; $C_{12}H_{12}O_2$ requires C, 76·6; H, 6·4%). It is highly soluble in ether, alcohol, benzene, ethyl acetate and aqueous alkali but sparingly so in petroleum ether. It does not give any colour with alcoholic ferric chloride. It dissolves in conc. sulphuric acid to give a yellow solution.

Menaphthone (2-*Methyl*-1 : 4-*naphthoquinone*) (VI)

1-Hydroxy-2-methyl-4-methoxy naphthalene (1 g.) was dissolved in the minimum quantity of ether and fuming nitric acid (1 c.c.) added. The resulting red solution was shaken well for two hours and the ether was removed. On diluting the solution with water and cooling, it deposited a colourless crystalline mass (0·75 g.). It was filtered, washed with water and dried in a vacuum desiccator. It crystallised from petroleum ether as small light yellow needles melting at 104–06°. It dissolves in sulphuric acid to give a red solution. With sodium ethoxide, it gives a transient blue

colour and then a stable reddish brown colour. When it is added to a solution of 2:4-dinitro-phenylhydrazine in hydrochloric acid followed by ammonia and the whole solution diluted with water, a stable green colour is obtained. On reductive acetylation, it gives a compound which melts at 113–14°. All these tests agree with those recorded for menaphthone in the literature.

1:4-*Dihydroxy-2-naphthaldehyde*

This was obtained from α-naphthohydroquinone by Gatterman's method using hydrogen cyanide and zinc chloride in ten per cent. yield.[15] The hexamine condensation of 1:4-dihydroxy-naphthalene was also carried out in the same manner as with the quinol monomethyl ether but the aldehyde was obtained in very poor yield (1%). The use of inert atmosphere like carbon-dioxide for the condensation did not improve the yield.

2-*Methyl-α naphthohydroquinone*

Clemmensen reduction of the above quinol aldehyde using the same procedure and quantities of reagents as in the case of 1-hydroxy-4-methoxy-2-naphthaldehyde gave 2-methyl-α-naphthohydroquinone in ten per cent. yield. It crystallised from dilute alcohol as colourless needles melting at 160–61°.

Menaphthone (*VI*)

2-Methyl-α- naphthohydroquinone (1 g.) was dissolved in ether (15 c.c.) and nitric acid (*d*, 1·2; 5 c.c.) added to it. The mixture was shaken well for one and a half hours; ether was removed and the solution diluted with water when menaphthone separated as a pale yellow crystalline solid (0·8 g.). It crystallised from ligroin as pale yellow needles melting at 105–16°.

Lawsone (*VII*)

(*a*) *Oxidation of* 1-*hydroxy*-4-*methoxy*-2-*naphthaldehyde*.—The aldehyde (1 g.) was dissolved in 4% aqueous sodium hydroxide (6 c.c.) and pyridine (50 c.c.), cooled in ice and treated with 5% hydrogen peroxide (10 c.c.) little by little during the course of fifteen minutes, with simultaneous shaking of the resulting deep red solution. The shaking was continued for another fifteen minutes and the solution left in ice-cold water-bath. After two hours, it was neutralised, extracted with ether and the ethereal layer dried over anhydrous sodium sulphate. On evaporating the ether, fine yellow needles separated out. These were filtered, washed with a little ether and dried (yield, 0·5 g.). The substance crystallised from dilute alcohol in

glistening yellow needles melting at 194–98° with decomposition. It turned red on keeping for a while in air. It dissolved in aqueous sodium bicarbonate, sodium carbonate, ammonia, lime water and sulphuric acid to give orange-red solutions. With alcoholic ferric chloride it gave a reddish brown colour. Reductive acetylation gave a product melting at 134°. The acetyl derivative obtained by heating it with acetic anhydride and a drop of sulphuric acid on a water-bath melted at 128–29°. In all these properties and reactions it agrees with lawsone as described in the literature.[16]

(*b*) *Oxidation of* 1 : 4-*dihydroxy*-2-*naphthaldehyde*.—The quinol aldehyde was subjected to Dakin's reaction, following the procedure already given and taking the same quantities of reagents, pyridine being omitted. The product crystallised from dilute alcohol as fine reddish yellow needles, m.p. 194–8°, and it was identical with the above sample of lawsone.

(*c*) *Oxidation of* 1 : 4-*dihydroxy*-2-*acetyl naphthalene* (*IX*).—The ketone was prepared by persulphate oxidation of 1-hydroxy-2-acetyl naphthalene (VIII), following the procedure of Desai and Sethna.[4] It was treated with hydrogen peroxide and alkali as in the last experiment. In this experiment, immediately after acidification, lawsone precipitated out as a red crystalline solid which was filtered, washed with water and crystallised from dilute alcohol, when it came out as small glistening yellow needles, melting at 194–8° with decomposition. Ether extraction of the mother-liquor provided more of lawsone (total yield, 50–60%).

(*d*) (i) *Preparation of* 1-*hydroxy*-4-*methoxy*-2-*acetyl naphthalene* (*X*).—2-Acetyl-α-naphthohydroquinone (IX) was partially methylated under dry conditions as follows: A mixture of the ketone (2 g.), dimethyl sulphate (1 c.c.), benzene (100 c.c.) and potassium carbonate (5 g.) was refluxed on a water-bath for 18 hours. Water was then added to dissolve potassium salts and the benzene layer separated. It was washed with sodium carbonate solution three times and then extracted exhaustively with five per cent. alkali. The alkaline solution was cooled, acidified with hydrochloric acid and the precipitated compound was filtered, washed with water and dried. It crystallised from ethyl acetate-ligroin as golden yellow stout rcetangular prisms melting at 121°. It dissolves in alcohol, benzene, ethyl acetate but is insoluble in wtaer. It dissolves in sodium hydroxide to give a yellow solution. With alcoholic ferric chloride it gives an intense green colour (Found: C, 72·5; H, 5·9; $C_{13}H_{12}O_3$ requires C, 72·2; H, 5·5%).

(*d*) (ii) *Oxidation*.—The above ketone on being subjected to Dakin's reaction as in the case of 1-hydroxy-4-methoxy-2-naphthaldehyde gave lawsone in 35–40% yield.

Summary

Based on biogenetic considerations new syntheses of menaphthone and lawsone are given. From α-naphthol, 1-hydroxy-4-methoxy-2-naphthaldehyde is prepared. This undergoes Clemmensen reduction and subsequent oxidative demethylation with nitric acid to yield menaphthone. On the other hand, Dakin's oxidation gives directly lawsone and this change involves oxidative demethylation by hydrogen peroxide in alkaline solution. A convenient laboratory method for preparing lawsone employs 2-acetyl-α-naphthohydroquinone.

Note added in Proof.—Recently we came across the following references in the literature: (i) Synthesis of menaphthone by Pavolini, *Recerca Sci.*, 1948, **18**, 134–8. Starting with naphthalene and passing through 6 stages he has reported an over all yield of 3·5% of the final product. His procedure is different from ours. (ii) Synthesis of Lawsone by Molho and Mentzer, *Experientia*, 1950, **6**, 11–12. These authors claim the formation in very low yields of lawsone from 2-methoxy naphthalene by oxidation with chromic acid or lead tetra-acetate and subsequent-demethylation. Better yields are claimed by the oxidation of α-naphthol with alkaline hydrogen peroxide.

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A STUDY OF APIIN FROM THE PARSLEY SEEDS AND PLANT

By S. R. Gupta and T. R. Seshadri, F.A.Sc.
(From the Department of Chemistry, Delhi University)

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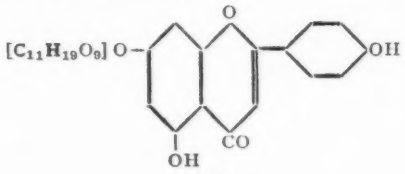
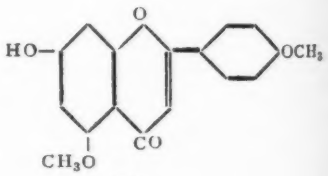
Before the synthetic dyestuffs industry developed, anthoxanthins were commonly employed as mordant dyes and many vegetable sources containing them were successfully used for this purpose. More recently it has been discovered that they have important physiological effects on the animal system.[1] Hence careful account should be taken of their presence in various food materials. Among them the parsley plant is known to contain a considerable amount of anthoxanthin. A number of earlier workers noted the presence of the glycoside, apiin, in the seeds, leaves and stems of parsley. This was first obtained in the crystalline condition by Lindenhorn[2] and was shown by von Gerichten[3] to be a glycoside of apigenin. Apiin is of special interest because it contains as a component sugar, a branched chain pentose, apiose; it is an apiose glucoside of apigenin. The position of the disaccharose unit could be surmised from the earlier results on partial methylation of apiin and its hydrolysis. It was unequivocally established by the experiments of Narasimhachari and Seshadri[4] by complete methylation and hydrolysis whereby 5:4′-dimethyl apigenin (II) was obtained as the product, thus proving that the 7-position was involved in the linkage with the sugar unit (I).



(I)



(II)

Considerable difficulty was experienced by earlier workers in getting apiin in a crystalline condition. A successful method adopted by Perkin[5] was as follows: To water kept continually boiling the apiin was added so as to form a strong solution and the yellow liquid very rapidly concentrated until a semi-solid, crystalline mass was obtained; this was collected while hot with the aid of the pump, washed with a little hot water and finally

pressed, these operations being performed with rapidity. Obtained in this way it forms a colourless mass of fine silky needles. But this procedure is not convenient to carry out and does not always give a crystalline and non-sticky product. Further, no data has been available for quickly characterising apiin. Its melting point was reported to be 228° but its acetyl derivative was not prepared and characterised. It was, therefore, felt necessary to get more information about apiin. First a convenient method of crystallising this glycoside has now been worked out. The chief impurity in apiin, which is very difficult to remove, seems to be of carbohydrate nature. By the conversion of crude apiin into a lead salt and subsequent recovery of apiin, it is found possible to effect its purification. On adding neutral lead acetate to an aqueous solution of crude apiin, a small amount of a greenish yellow precipitate is formed; it is discarded because it does not yield any crystalline product on working up. Subsequent addition of basic lead acetate gives a bulky yellow precipitate from which hydrogen sulphide liberates apiin which then crystallises readily from alcohol. This product melts at 230–2° and also forms a crystalline acetate melting at 249–51°.

In the earlier work of Narasimhachari and Seshadri[4] complete methylation of apiin and hydrolysis gave a dimethyl ether of apigenin whose melting point was found to be 265–7°. The same melting point had also been recorded by Zemplen *et al.*[6] for the dimethyl ether obtained from linarin. This substance was also obtained by the oxidation of naringin with iodine and sodium acetate followed by complete methylation and hydrolysis.[4] Its properties agreed with the given constitution and there seemed to be little doubt because of the agreement in the properties of the product obtained from a number of sources. More recently Baker, Hemming and Ollis[7] in connection with their work on buddleoflavonoloside obtained 5 : 4′-dimethyl apigenin having the melting point as 298°. They also expressed the opinion that the earlier preparations of the compound might have been impure. This discrepancy could be due to (i) the use of not completely purified apiin yielding impure dimethyl apigenin or (ii) the capacity of the product of exhiibting dual melting point and hence there was need for the reinvestigation of this question. The dimethyl apigenin sample melting at 265–7° did not improve after repeated recrystallisation. In order to see if this was due to the presence of a persistent impurity which could not be removed by simple crystallisation, acetylation was made. This gave rise to an acetyl derivative whose melting point agreed with that reported by Baker *et al.*[7] for the acetate of 5 : 4′-dimethyl apigenin. When the acetate was hydrolysed the resulting apigenin dimethyl ether melted at 297–98° agreeing with the melting point reported by the above authors. In another experiment

crystalline apiin was fully methylated with excess of dimethyl sulphate and potassium carbonate in anhydrous acetone medium till the product gave no colour with ferric chloride, the methyl ether of the glycoside was purified and then hydrolysed. The resulting dimethyl apigenin gave no difficulty in purification and melted at 297–8°. Thus the lower melting point recorded earlier was due to the presence of a persistent impurity.

Von Gerichten[8] in his study of the parsley plant using leaves and stems reported that it contained two glycosides. He hydrolysed the mixture and obtained from the product both apigenin and diosmetin. He, therefore, concluded that the original glycoside mixture consisted of apiin and the corresponding glycoside of diosmetin. He does not appear to have isolated apiin itself from the plant. Using seeds provided by Carters, London and described as 'Carters Champion Moss Curled' parsley plants were raised in Delhi and in the fresh condition were extracted and studied for the presence of the glycosides. The crude product could be separated into two fractions by treatment with cold acetone. The undissolved portion, when purified by the lead acetate method, readily yielded pure apiin melting at 230–2° and forming an acetate melting at 249–51°. These were identical with the samples obtained from parsley seeds and the identity was established by taking mixed melting points. Therefore there is no doubt that the parsley plant also contains apiin. The acetone-soluble portion when similarly purified using the lead salt method gave a product melting at 218–20°. Though the melting point was lower its reactions were similar to those of apiin. On acetylation it formed an acetate melting at 249–51° and identical with apiin acetate. The mixed melting point was undepressed. Thus there seemed to be no other glycosidic substance in the extract except apiin. Even the colour of the lead salt seemed to indicate that there was no significant amount of diosmetin glycoside. This result is different from that of von Gerichten[8] who reported to have obtained almost equal quantities of apigenin and diosmetin in his extraction of the parsley plant. This chemical difference may probably be accounted for as due to varietal differences in the parsley plant used for the experiments or due to the effect of climate.

EXPERIMENTAL

Isolation of Apiin from Parsley Seeds.—Air-dried powdered seeds of parsley (600 g.) were soaked in petroleum ether. After 24 hours the extract was decanted off. Two such extractions with this solvent removed most of the essential oils, fatty and waxy matter. Then the seeds were extracted first with cold alcohol (12 hours) and finally with boiling alcohol twice, each hot extraction taking 6 hours. The combined alcoholic extract was con-

centrated to small bulk under diminished pressure and cooled when a thick gelatinous mass separated. Crude apiin was obtained as a fine yellow powder by extracting the above gelatinous mass with ether in order to remove chlorophyll, fatty matter and any free flavone that might be present. Yield, 13·0 g. (2·2%).

Purification and Crystallisation of Apiin.—The above sample of apiin could not be crystallised from alcohol. It separated as a gelatinous mass when its hot alcoholic solution was cooled. It was purified in the following manner: To a boiling aqueous solution of the crude apiin (4 g.) a solution of neutral lead acetate was added dropwise till no more precipitate was formed and the mixture filtered hot. The greenish yellow precipitate which was very small in quantity was rejected. A solution of basic lead acetate was added to the filtrate till no more precipitate separated. The bulky yellow lead salt was filtered and while still wet was ground up and suspended in ethanol and hydrogen sulphide was passed into the supension till the decomposition was complete. The precipitatate of lead sulphide was filtered off. After boiling off hydrogen sulphide the alcoholic filtrate was kept overnight when a cream coloured crystalline aggregate of apiin (2 g.) separated out. On recrystallising from alcohol it was obtained as colourless needles melting at 230–32° (m.p. given by von Gerichten[3] 228°). In alcoholic solution apiin gives a brown colour with ferric chloride and it dissolves in 1% sodium hydroxide and carbonate to form yellow solutions. A 0·5% aqueous solution of apiin containing 0·2% of potassium hydroxide was employed for determining specific rotation; α_D^{20}, −130°. (Found: C, 53·8; H, 5·1; $C_{26}H_{28}O_{14}$, H_2O requires C, 53·6; H, 5·2%).

Apiin Acetate.—Apiin (0·7 g.), anhydrous pyridine (2 c.c.) and acetic anhydride (10 c.c.) were refluxed in an oil-bath at 140–50° for 3 hours, cooled and poured over crushed ice. The solid product was collected, washed and dried (0·8 g.). It was found to be sparingly soluble in alcohol. It crystallised from acetone as aggregates of colourless needles and melted at 249–51°, unaltered by further crystallisations. (Found: C, 55·4; H, 4·6; $C_{42}H_{44}O_{22}$ requires C, 56·0; H, 4·9%.)

Hydrolysis.—Crystalline apiin (0·5 g.) was refluxed with 7% aqueous sulphuric acid (100 c.c.) for 2 hours. Yellow aglucone started separating out even after half an hour. It was filtered and crystallised from aqueous pyridine; yellow needles, m.p. 343–5°. Kostanecki *et al.*[9] give m.p. of apigenin as 347–8°. Yield, 0·2 g. It was acetylated using acetic anhydride and pyridine. The acetate (0·1 g.) crystallised from alcohol as colourless needles melting at 181–2° agreeing with the melting point of apigenin triacetate described in the literature.[9]

Partial Methylation of Apiin and Hydrolysis (*Acacetin*).—Crystalline apiin (0·5 g.) was made into fine suspension in dry acetone (150 c.c.) and dimethyl sulphate (0·1 c.c.) and anhydrous potassium carbonate (2 g.) were added and the mixture refluxed for 15 hours. It was then filtered and the potassium salts (R) washed with hot acetone. On distilling off the solvent from the filtrate a viscous semi-solid was obtained. It was directly hydrolysed by boiling with 7% aqueous sulphuric acid for 2 hours when a pale yellow aglucone separated.

The potassium salts residue (R) was found to contain further quantities of the methylated glycoside. On dissolving it in water and adding sufficient quantity of sulphuric acid not only to neutralise the carbonate but also to raise the acid concentration to 7% and heating under refluex for 2 hours, a pale yellow solid was obtained. Combined yield, 0·1 g. It crystallised from aqueous pyridine in the form of colourless needles melting at 257–8° and was identical with an authentic sample of acacetin.

Complete Methylation of Apiin and Hydrolysis.—A fine suspension of crystalline apiin (2 g.) in dry acetone (150 c.c.) was methylated by refluxing with an excess of dimethyl sulphate and anhydrous potassium carbonate for 60 hours. It was then filtered and the potassium salts washed with hot acetone. On distilling off the solvent from the filtrate a yellow sticky mass separated. The excess of dimethyl sulphate was removed by washing the methylated product a number of times with petroleum ether. The product so obtained was dissolved in the minimum amount of boiling acetone. The dimethyl ether of apiin was precipitated out by the addition of excess of petroleum ether. After decanting off the acetone-petroleum ether mixture the precipitated apiin dimethyl ether was dissolved in alcohol. From the alcoholic solution, the methylated glycoside separated as a white gelatinous mass which on subsequent filtration and drying melted at 145–50°. It gave no colour with alcoholic ferric chloride solution.

The methylated glycoside (1·5 g.) was hydrolysed with 7% aqueous sulphuric acid when a yellow solid separated out. The product crystallised from alcohol as colourless rectangular prisms melting at 297–8° d. It dissolved in aqueous sodium hydroxide giving a yellow solution. Its alcoholic solution gave no colour with ferric chloride.

The impure dimethyl ether of aglucone melting at 265–7°[4] was acetylated using acetic anhydride and dry pyridine. The 7-acetoxy-5:4′-dimethoxy flavone crystallised from ethyl acetate-absolute alcohol mixture as colourless needles melting at 149–51° (identical with the melting point reported by Baker *et al.*[7]). It was deacetylated by heating with alcohol and hydro-

chloric acid (1 : 1) for 20 minutes over a boiling water-bath. The product crystallised from alcohol as rectangular prisms melting at 297–8°.

Extraction of the Parsley Plant.—Fresh stems and leaves of parsley (29 lb.) were cut into small pieces and extracted twice by keeping them immersed in cold ethyl alcohol for 48 hours each time. Final extraction was effected by heating under reflux with alcohol for 6 hours on a water-bath. Most of the alcohol was distilled off under diminished pressure from the combined alcoholic extract (10 litres) and the concentrated solution filtered hot under suction in order to remove some sticky greenish impurity. On cooling the filtrate, a thick greenish gelatinous mass separated out. It was filtered from the mother-liquor (M) and extracted with cold ether to dissolve out chlorophyll and fatty matter. The resulting solid product was extracted with cold acetone and filtered. The undissolved fraction was marked (A). On distilling off acetone from the filtrate was obtained the more soluble fraction (B). It was a semi-solid mass which was dried and subsequently extracted with ether. It then became a definite solid.

By concentrating the mother-liquor (M) in stages till final evaporation further fractions of solid were obtained. They were also extracted with ether and separated using acetone into two fractions which were added to A and B respectively. Total yield of (A) was 75 g. and of (B) 30 g.

Purification of Fraction (A).—The crude glycoside (2 g.) was purified by means of lead acetate as described in the case of apiin from the seeds. The behaviour of the sample was exactly the same. The crystalline glycoside melted at 230–2°. Yield, 0·8 g. The mixed melting point with the authentic sample of apiin obtained from the seeds was undepressed. It gave a brown colour with alcoholic ferric chloride and dissolved in 1% sodium carbonate to form a yellow solution. A 0·5% solution of this glycoside containing 2% potassium hydroxide gave a specific rotation of −130°. This was acetylated with acetic anhydride and pyridine and the acetate melted at 249–51°. The mixed melting point with apiin acetate from the seeds was undepressed.

Purification of Fraction (B).—The procedure adopted for the purification of this fraction was exactly similar to the one employed above. The decomposition of the basic lead acetate fraction with hydrogen sulphide gave a crystalline substance melting at 218–20° with sintering a few degrees earlier. The melting point was unaltered on recrystallisation from alcohol. An alcoholic solution of the compound gave a brown colour with alcoholic ferric chloride and dissolved in sodium carbonate solution giving a yellow colour. A mixture of this with the apiin from the seeds melted between

220 and 230°; there was no depression. Acetylation of this glycoside was carried out just as in the previous cases using acetic anhydride and pyridine. The acetate crystallised from acetone as aggregate of colourless fibrous needles and melted at 249–51°. The mixed melting point with the authentic sample of apiin acetate was undepressed.

SUMMARY

An effective method for purifying apiin from parsley seeds is to convert it into the lead salt and recover it by decomposition with hydrogen sulphide. It then crystallises readily from alcohol and yields a crystalline acetate. The work on the complete methylation and hydrolysis has been revised using the pure sample and also purifying the methylated glycoside obtained as intermediate. The resulting 5 : 4′-*o*-dimethyl apigenin is found to melt correctly at 297–8° as mentioned by Baker *et al.* Even the impure sample obtained earlier from crude apiin can be purified through its acetate, and then its melting point is found to be higher as mentioned above.

Extraction of the parsley plant grown in Delhi yielded only apiin as the anthoxanthin component and the presence of luteolin glycoside reported by von Gerichten could not be detected.

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THE INFRA-RED ABSORPTION SPECTRUM OF POTASSIUM CHLORATE CRYSTALS: PART I

By A. K. Ramdas

(From the Raman Research Institute, Bangalore)

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1. Introduction

The infra-red spectrum of potassium chlorate was first investigated by Schæfer and Schubert (1921) using pressed powder and employing the restrahlen method. They reported two reflection maxima at $10 \cdot 12\,\mu$ (988 cm.$^{-1}$) and $16 \cdot 12\,\mu$ (620 cm.$^{-1}$) respectively. Subsequently, several studies have been published of the Raman effect in the substance in solution, as crystal powder and also as a single crystal. It is proposed in this paper to report the results of the investigation of the infra-red absorption spectrum of thin single crystals of potassium chlorate, made by the transmission method, using a Beckman infra-red spectrophotometer (Model IR 2) in the range between $1\,\mu$ to $15\,\mu$ provided by a dispersing prism of potassium bromide.

Single crystals of potassium chlorate were obtained from a solution of the pure substance in water by slow evaporation. The crystals are formed as plates parallel to the 001 plane. Three crystals were examined. One of them (about $5 \times 5 \times 1$ mm. size) was studied in detail, readings being taken at intervals of $0 \cdot 25\,\mu$, and at still closer intervals near the absorption maxima. The other two plates were examined less closely, readings being taken at intervals of $0 \cdot 5\,\mu$. But as these specimens were thinner than that examined in greater detail, they exhibit a clearer resolution of some of the broad absorption bands. The crystal was interposed with its flat face perpendicular to the infra-red radiation, the percentage transmission being read off directly with the instrument.

Figs. 1 and 2 exhibit the percentage cut-off for the different wavelengths investigated. Fig. 1 gives the results with the specimen examined in detail, while Fig. 2 gives the results obtained with a thinner specimen.

Table I gives the position of the absorption bands observed in this investigation. For comparison with the same, the reflexion maxima reported by Schæfar and Schubert, the results of Shantakumari on the Raman effect

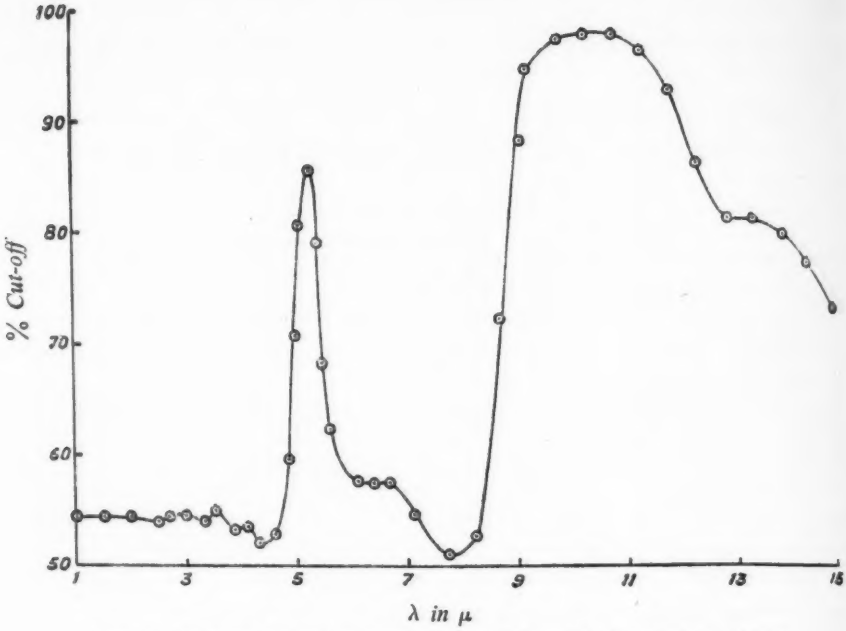

FIG. 1. Infra-red absorption spectrum of single crystal of potassium chlorate (thickness about 1 mm.)

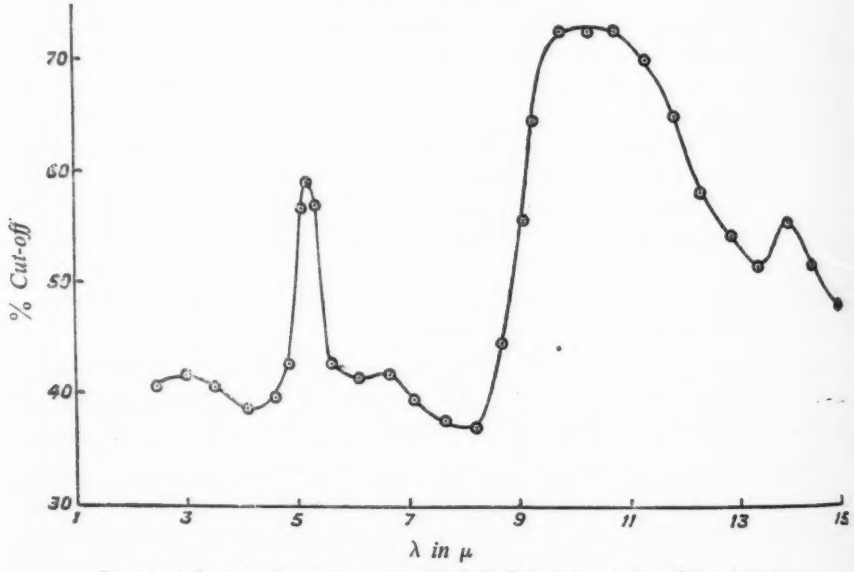

FIG. 2. Infra-red absorption spectrum of single crystal of potassium chlorate (thickness < 1 mm.)

in single crystals of potassium chlorate and of Venkateswaran on the Raman effect in solution are also tabulated.

TABLE I

Infra-red and Raman Spectra of $KClO_3$

Infra-red Absorption Bands (*a*)			Infra-red Restrahlen (*b*)		Raman effect single crystal (*c*)		Raman effect in solution (*d*)	
μ	cm.$^{-1}$	Description	μ	cm.$^{-1}$	μ	cm.$^{-1}$	μ	cm.$^{-1}$
2·85	3509	Weak						
3·5	2857							
4·1	2439							
5·3	1887	Strong and sharp						
6·7	1493	Weak						
9·2	1087	Strong, broad	10·12	988	10·26	975(7)	10·24	977(1)
↓	↓				10·75	930(10)	10·75	930(10)
12·0	833				10·87	920(1)		
12·8	781	Weak						
↓	↓							
13·6	735							
			16·12	620	16·12	620	?	
					20·58	486(6)	20·92	478(4)
					73·53	136(4)		
					102·0	98(5)		
					122·0	82(3)		
					185·2	54(3)		

a—Author, *b*—Schæfer-Schubert (1921), *c*—Shantakumari (1950), *d*—Venkateswaran (1938).

It will be noticed from the figures that a well-defined infra-red absorption band is observed with its maximum located at 5·3 μ, while on the other hand there is a very broad band covering the region between 9·2 μ to 12 μ. Other and less prominent features are also noticeable, *viz.*, a subsidiary absorption band with its maximum at about 6·7 μ and another at about 13·5 μ.

2. Discussion of the Results

The experimental data for the Raman effect in potassium chlorate crystal and in solution exhibit the characteristic frequencies of the ClO_3^- group in nearly the same positions; the relative intensities of the lines, however, show differences. We shall come to this point a little later. It is well established that the chlorate ion in the free state has a pyramidal structure with chlorine at the apex, with the symmetry of the point group C_{3v}.

Accordingly, the free ion possesses two totally symmetric (A_1) vibrational modes and two doubly degenerate ones (E). All the modes are permitted both in infra-red and Raman effect. The totally symmetric vibrations should give polarised Raman lines ($\rho < \frac{6}{7}$) while the doubly degenerate lines are depolarised ($\rho = \frac{6}{7}$). By polarisation studies of the Raman lines of the chlorate ion Shen, Yao and Wu (1937) have classified them as follows:

TABLE II

Classification of the Raman Lines of the ClO_3^- Ion

	cm.$^{-1}$	μ	ρ	Class
ν_1	930	10·75	0·35	A_1
ν_2	975	10·26	6/7	E
ν_3	620	16·12	0·56	A_1
ν_4	486	20·58	6/7	E

The selection rules allow the combinations and the overtones of all the fundamental oscillations in Raman effect and infra-red.

In addition to the high frequency internal oscillations of the ClO_3^- ion as modified by the interactions of the surrounding K^+ ions, low frequency lattice oscillations will occur in the crystal of potassium chlorate. The crystal belongs to the monoclinic prismatic class, and contains two molecules per unit cell, its space group being C^2_{2h}. The group-theoretical analysis shows that there should be nine Raman-active lattice oscillations and six infra-red-active oscillations, the two sets being mutually exclusive. Shantakumari has recorded five lattice oscillations in Raman effect.

The lattice oscillations are of low frequencies and lie outside the range of the spectrophotometer used in this work. The frequencies ν_3 and ν_4 also lie out of the range investigated. But the combinations and overtones of these internal frequencies will occur within the experimental range. Similarly, one may expect to find difference as well as combination lines between the lattice and internal vibrations. In the light of these remarks, one may interpret the experimentally observed absorption bands as shown in Table III.

Besides the principal absorption frequencies ν_1 and ν_2, the various combinations $\nu_1 \pm L$, $\nu_2 \pm L$, where L represents a lattice vibration frequency are also possible, and the presence of such combinational absorptions may

TABLE III

Observed absorption maxima		Assignment	Calculated	
$\lambda\mu$	cm.$^{-1}$		$\lambda\mu$	cm.$^{-1}$
5·3	1887	$2\nu_1$	5·38	1860
		$\nu_1+\nu_2$	5·25	1905
		$2\nu_2$	5·13	1950
6·7	1493	$\nu_1+\nu_3$	6·45	1550
		$\nu_2+\nu_4$	6·84	1461
9·2	1087	ν_2	10·26	975
↓	↓	$2\nu_4$	10·29	972
12	833	ν_1	10·75	930

partly or wholly be responsible for the notable width of the band covering the range between 9 μ and 12 μ.

As remarked earlier, the internal frequencies of $KClO_3$ show remarkable changes of intensity in the Raman effect as we pass from liquid to crystalline state. For example, the frequencies ν_2, 977 (1), and ν_1, 930 (10) in solution become ν_2, 975 (7) and ν_1, 930 (10) in the single crystal. In the infra-red restrahlen of the pressed powder as observed by Schæfer and Schubert, 975 cm.$^{-1}$ comes out much stronger than 930 cm^{-1}. In the present work, both the frequencies ν_1 and ν_2 seem to have come out with more or less equal intensities, as fundamentals and also as octaves.

The behaviour of sodium chlorate affords some interesting comparisons with potassium chlorate. In Raman effect in $NaClO_3$ solution studied by Venkateswaran (1938), ν_1, 927 (10) appears much stronger than ν_2, 971 (2). Even in the Raman effect in a single crystal of $NaClO_3$ as studied by Chandrasekharan (1950) in different settings, the lines 933–36 are very much stronger than the 966–84 lines. On the other hand, in the restrahlen studies with $NaClO_3$ crystal made by Schæfer and Schubert, 966–84 lines appear more strong than 933–36 lines, the latter being noticeable as a weak wing.

Potassium chlorate has a highly anisotropic structure and the specific orientations of the crystal may therefore be expected to influence its behaviour. It appears therefore not unlikely that the manifestation of ν_1 and ν_2 with nearly equal intensity, both in this investigation as well as in the Raman effect study with a single crystal of $KClO_3$ by Shantakumari, is a consequence of the particular orientation of the crystal with which these studies

were made. Further studies are, however, needed to establish whether this is the actual explanation of the striking differences in the relative intensity of ν_1 and ν_2 as between the chlorates of sodium and potassium observed in respect of both infra-red and Raman activities.

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3. SUMMARY

The infra-red transmission through the 001 face of a single crystal of potassium chlorate reveals, besides a broad absorption band in the range $9{\cdot}2\,\mu$ to $12\,\mu$, a second and narrower band with its maximum at $5{\cdot}3\,\mu$. The former band can be explained as due to the infra-red activity of the vibration frequencies ν_1 (930 cm.$^{-1}$) and ν_2 (975 cm.$^{-1}$) of the crystal also observed in the Raman effect, and their combinations with the low frequency lattice oscillations. The band at $5{\cdot}3\,\mu$ may likewise be explained as due to the infra-red activity of the octaves of ν_1 and ν_2 and of their summational frequency.

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ON THE FIERZ-PAULI EQUATION FOR PARTICLES OF SPIN 3/2

By K. K. Gupta

(Tata Institute of Fundamental Research, Bombay)

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§1

Bhabha (1949) has shown that every equation for an elementary particle of finite mass can be written in the form

$$(p_k a^k + \chi)\,\psi = 0, \tag{1}$$

where $p_k = -i\,\frac{\partial}{\partial x^k}$, $(x^0,\ x^1,\ x^2,\ x^3 = ct,\ x,\ y,\ z)$; a^k are $\nu \times \nu$ matrices defining the spin; χ a constant; and the wave function ψ a $\nu \times 1$ matrix defining the state of the particle. He has shown that the values of the rest mass of the particle are determined by the minimal equation of the a-matrices. In particular, when components of ψ satisfy the second order equation a^0 must satisfy the minimal equation

$$\{(a^0)^2 - 1\}\,(a^0)^s = 0, \tag{2}$$

where $s \geqslant 0$ is an integer.

When the four a^k form an irreducible set, the generators I^{kl} of the representation R of the Lorentz group in four dimensions according to which the wave function ψ transforms, are connected with the a^k by the following relation (Harish-Chandra, 1947):

$$\mathrm{I}^{kl} = \Sigma\,\mathrm{A}\,(a \ldots a^k \ldots a^l \ldots a - \ ), \tag{3}$$

where the dots stand for an unspecified number of a's the index of each such a being contracted with that of another a in the same term. The minus sign denotes that the same terms with k and l interchanged are to be subtracted.

We shall here write down the equations of Fierz and Pauli (1939) for a particle of spin 3/2 in the canonical form (1) and obtain the commutation relations for the corresponding a^k's. We shall also investigate the relation between 1^{kl} and a^i. This relation cannot be

$$\mathrm{I}^{kl} = a^k a^l - a^l a^k \tag{4}$$

for Bhabha has investigated all equations of the type (1) in which this relation holds, and shown that for all except the well-known cases of spin 0, $\frac{1}{2}$, and 1, namely the Klein-Gordon, the Dirac, and the Proca equations, the particle has more than one value of the rest mass. Since the particle has only one rest mass for the Fierz-Pauli equations the relation (3) cannot hold.

§ 2

The Dirac (1936) equations for a particle of spin 3/2 are

$$p^{\dot{\beta}\rho}\, a^{\dot{\alpha}}_{\rho\gamma} + p^{\dot{\alpha}\rho}\, a^{\dot{\beta}}_{\rho\gamma} = 2\chi b^{\dot{\alpha}\dot{\beta}}_{\gamma} \tag{4a}$$

$$p_{\beta\dot{\alpha}}\, b^{\dot{\alpha}\dot{\beta}}_{\gamma} + p_{\gamma\dot{\alpha}}\, b^{\dot{\alpha}\dot{\beta}}_{\beta} = 2\chi a^{\dot{\beta}}_{\beta\gamma} \tag{4b}$$

with the subsidiary conditions:

$$p^{\rho}_{\dot{\alpha}}\, a^{\dot{\alpha}}_{\rho\gamma} = 0 \tag{5a}$$

$$p^{\beta}_{\dot{\alpha}}\, b^{\dot{\alpha}\dot{\rho}}_{\beta} = 0 \tag{5b}$$

where $a^{\dot{\alpha}}_{\rho\gamma}$, $b^{\dot{\alpha}\dot{\beta}}_{\gamma}$ are spinors, the spinor indices running through 1, 2, and $\dot{1}$, $\dot{2}$. $p_{\beta\dot{\alpha}} = \sum_{k=0}^{3} p_k \sigma^{k}_{\beta\dot{\alpha}}$ with

$$\sigma^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

the indices β and $\dot{\alpha}$ denoting the row and column of the matrices respectively; χ is a constant related to the mass of the particle. Summation over indices occurring both above and below in the same term is understood throughout this paper. With the help of (2) one can easily see from (1) that the wave functions $a^{\dot{\alpha}}_{\rho\gamma}$ and $b^{\dot{\alpha}\dot{\beta}}_{\gamma}$ satisfy the second order equation.

Equations (4) and (5) cannot be obtained by the variation of a Lagrange function as they stand. To make this possible, Fierz and Pauli (1939)

introduced subsidiary spinors c_μ, $d^{\dot\mu}$ and obtained equations by the variation of a Lagrangian which lead back to equations (4) and (5). They took

$$\mathrm{L} = \chi\left\{a^{*\gamma}_{\alpha\beta\cdot}\, b^{\alpha\dot\beta}_{\gamma} + b^{*\beta\alpha}_{\gamma\cdot}\, a^{\dot\gamma}_{\alpha\beta}\right\} - \left\{a^{*\gamma}_{\alpha\beta\cdot}\, p^{\dot\beta\rho}\, a^{\dot\alpha}_{\gamma\rho} + b^{*\alpha\beta}_{\gamma\cdot}\, p_{\alpha\rho\cdot}\, b^{\dot\gamma\dot\rho}_{\beta}\right\}$$

$$- \left\{a^{*\gamma}_{\alpha\beta\cdot}\, p^{\dot\beta}_{\gamma}\, d^{\dot\alpha} + b^{*\alpha\beta}_{\gamma\cdot}\, p^{\dot\gamma}_{\beta}\, c_\alpha + \text{complex conjugate}\right\}$$

$$+ 6\chi\left\{d^{*\alpha}\, c_\alpha + d^{\dot\alpha}\, c^{*}_{\alpha\cdot}\right\} + 3\left\{d^{*\alpha}\, p_{\alpha\dot\beta\cdot}\, d^{\dot\beta} + c^{*}_{\alpha\cdot}\, p^{\dot\alpha\beta}\, c_\beta\right\} \qquad (6)$$

Variation of L gives:

$$2\chi b^{\dot\alpha\dot\beta}_{\gamma} - p^{\dot\beta\rho}\, a^{\dot\alpha}_{\gamma\rho} - p^{\dot\alpha\rho}\, a^{\dot\beta}_{\gamma\rho} - p^{\dot\beta}_{\gamma}\, d^{\dot\alpha} - p^{\dot\alpha}_{\gamma}\, d^{\dot\beta} = 0 \qquad (7a)$$

$$2\chi a^{\dot\gamma}_{\alpha\beta} - p_{\alpha\rho\cdot}\, b^{\dot\gamma\dot\rho}_{\beta} - p_{\beta\rho\cdot}\, b^{\dot\gamma\dot\rho}_{\alpha} - p^{\dot\gamma}_{\beta}\, c_\alpha - p^{\dot\gamma}_{\alpha}\, c_\beta = 0 \qquad (7b)$$

$$- p^{\beta}_{\gamma\cdot}\, a^{\dot\gamma}_{\alpha\beta} + 3p_{\alpha\beta\cdot}\, d^{\dot\beta} + 6\chi c_\alpha = 0 \qquad (7c)$$

$$- p^{\gamma}_{\beta\cdot}\, b^{\alpha\dot\beta}_{\gamma} + 3p^{\dot\alpha\beta}\, c_\beta + 6\chi d^{\dot\alpha} = 0 \qquad (7d)$$

from which one can derive equations (4), (5) and $c_\alpha = 0$, $d^{\dot\alpha} = 0$.

§ 3

Using the relations

$$p_{1\dot1} = p^{\dot2\dot2} = p_0 + p_3$$

$$p_{1\dot2} = -p^{\dot2\dot1} = p_1 - ip_2$$

$$p_{2\dot1} = -p^{\dot2\dot1} = p_1 + ip_2$$

$$p_{2\dot2} = \epsilon^{\dot1\dot1} = p_0 - p_3$$

write down the equations (7) explicitly in the form (1) with the following order for the components of ψ:

$$\psi = \begin{vmatrix} a_{11}^{1} \\ \sqrt{2}a_{12}^{1} \\ a_{22}^{1} \\ a_{11}^{2} \\ \sqrt{2}a_{12}^{2} \\ a_{22}^{2} \\ b_{1}^{11} \\ \sqrt{2}b_{1}^{12} \\ b_{1}^{22} \\ b_{2}^{11} \\ \sqrt{2}b_{2}^{12} \\ b_{2}^{22} \\ 3\sqrt{2}c_1 \\ 3\sqrt{2}c_2 \\ 3\sqrt{2}d^{1} \\ 3\sqrt{2}d^{2} \end{vmatrix} \tag{8}$$

The form of the matrices α^k can then be read directly. They are

$$\alpha^0 = \begin{pmatrix} 0 & u^0 & \frac{1}{3}v^0 & 0 \\ u^0 & 0 & 0 & -\frac{1}{3}v^0 \\ -w^0 & 0 & 0 & \frac{1}{2}\sigma^0 \\ 0 & w^0 & \frac{1}{2}\sigma^0 & 0 \end{pmatrix}, \tag{9a}$$

$$\alpha^k = \begin{pmatrix} 0 & u^k & \frac{1}{3}v^k & 0 \\ -u^k & 0 & 0 & \frac{1}{3}v^k \\ w^k & 0 & 0 & \frac{1}{2}\sigma^k \\ 0 & w^k & -\frac{1}{2}\sigma^k & 0 \end{pmatrix}, \quad k = 1, 2, 3, \tag{9b}$$

where

$$u^0=\begin{pmatrix} -1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & -\frac{1}{2} & \cdot & -\frac{1}{\sqrt{2}} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & -\frac{1}{\sqrt{2}} & \cdot \\ \cdot & -\frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & -\frac{1}{\sqrt{2}} & \cdot & -\frac{1}{2} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & -1 \end{pmatrix},$$

$$w^0=\begin{pmatrix} \cdot & -\frac{1}{2} & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot \\ \cdot & \cdot & -\frac{1}{\sqrt{2}} & \cdot & \frac{1}{2} & \cdot \end{pmatrix},$$

$$v^0=w^{0\dagger},\ \sigma^0=\begin{pmatrix} 1 & \cdot \\ \cdot & 1 \end{pmatrix};$$

$$u^1=\begin{pmatrix} \cdot & -\frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & \cdot \\ -\frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & -\frac{1}{2} & \cdot \\ \cdot & \cdot & \cdot & -1 & \cdot & \cdot \\ \cdot & \cdot & -1 & \cdot & \cdot & \cdot \\ \cdot & -\frac{1}{2} & \cdot & \cdot & \cdot & -\frac{1}{\sqrt{2}} \\ \cdot & \cdot & \cdot & \cdot & -\frac{1}{\sqrt{2}} & \cdot \end{pmatrix},$$

$$w^1=\begin{pmatrix} -\frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & \frac{1}{2} & \cdot \\ \cdot & -\frac{1}{2} & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} \end{pmatrix};$$

$$v^1=w^{1\dagger},\ \sigma^1=\begin{pmatrix} \cdot & 1 \\ 1 & \cdot \end{pmatrix},$$

$$u^2=\begin{pmatrix} \cdot & \frac{i}{\sqrt{2}} & \cdot & \cdot & \cdot & \cdot \\ -\frac{i}{\sqrt{2}} & \cdot & \cdot & \cdot & \frac{1}{2}i & \cdot \\ \cdot & \cdot & \cdot & -i & \cdot & \cdot \\ \cdot & \cdot & i & \cdot & \cdot & \cdot \\ \cdot & -\frac{1}{2}i & \cdot & \cdot & \cdot & \frac{i}{\sqrt{2}} \\ \cdot & \cdot & \cdot & \cdot & -\frac{i}{\sqrt{2}} & \cdot \end{pmatrix},$$

$$w^2=\begin{pmatrix} -\frac{i}{\sqrt{2}} & \cdot & \cdot & \cdot & -\frac{i}{2} & \cdot \\ \cdot & -\frac{i}{2} & \cdot & \cdot & \cdot & -\frac{i}{\sqrt{2}} \end{pmatrix}$$

$$v^2=w^{2\dagger},\ \sigma^2=\begin{pmatrix} \cdot & -i \\ i & \cdot \end{pmatrix};$$

$$u^3=\begin{pmatrix} -1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{2} & \cdot & -\frac{1}{\sqrt{2}} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot \\ \cdot & -\frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot & -\frac{1}{2} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix},$$

$$w^3=\begin{pmatrix} \cdot & \frac{1}{2} & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot \\ \cdot & \cdot & \frac{1}{\sqrt{2}} & \cdot & \frac{1}{2} & \cdot \end{pmatrix},$$

$$v^3 = w^{3\dagger},\ \sigma^3 = \begin{pmatrix} 1 & \cdot \\ \cdot & -1 \end{pmatrix}.$$

$\dagger$ denotes the Hermitian conjugate matrix. The matrices u^k are Hermitian.

We can construct a non-singular Hermitian matrix D such that $\mathrm{D}\alpha^k$ is Hermitian, *i.e.*,

$$\mathrm{D}\alpha^k = \alpha^{k\dagger}\,\mathrm{D}$$

and $\psi^\dagger \mathrm{D}\psi$ is invariant:

$$\mathrm{D} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{3} \\ 0 & 0 & \frac{1}{3} & 0 \end{pmatrix} \tag{10}$$

each element representing a block matrix as in the decomposition of the α^ks. For example

$$\mathrm{D}\alpha^0 = \begin{pmatrix} u & 0 & 0 & -\frac{1}{3}v \\ 0 & u & \frac{1}{3}v & 0 \\ 0 & \frac{1}{3}w & \frac{1}{6}\sigma^0 & 0 \\ -\frac{1}{3}w & 0 & 0 & \frac{1}{6}\sigma^0 \end{pmatrix}$$

which is obviously Hermitian.

By actual multiplication we can verify from (9*a*, *b*) that

$$\{(\alpha^0)^2 - 1)\}\,(\alpha^0)^2 = 0,$$

$$\{(\alpha^k)^2 + 1\}\,(\alpha^k)^2 = 0, \qquad k = 1, 2, 3.$$

in agreement with (2). These can be incorporated into the single relation

$$\{(\alpha^k)^2 - g^{kk}\}\,(\alpha^k)^2 = 0, \tag{11}$$

where

$$-g^{00} = g^{11} = g^{22} = g^{33} = -1,\ g^{kl} = 0 \text{ for } k \neq l.$$

We can now directly write down the commutation relations for different α^ks (*cf.*, Harish Chandra, 1947; Bhabha, 1949) from (11):

$$\sum_{\mathrm{P}} (\alpha^k \alpha^l - g^{kl})\,\alpha^m \alpha^n = 0. \tag{12}$$

where $\sum_{\mathrm{P}}$ stands for a sum over all permutations of the indices k, l, m, n. Since the algebra generated by matrices satisfying (12) cannot be finite, our α^ks must satisfy some additional algebraic relations compatible with (12).

§ 4

From the form (8) of ψ we see that the 16×16 representation R of the Lorentz group, according to which ψ transforms can be reduced to the following when one restricts oneself to the subgroup L_+ of proper Lorentz transformations:

$$R = \mathcal{D}_{1,\frac{1}{2}} + \mathcal{D}_{\frac{1}{2},1} + \mathcal{D}_{\frac{1}{2},0} + \mathcal{D}_{0,\frac{1}{2}}. \tag{13}$$

Correspondingly the generators I^{kl} of representation R will reduce to

$$I^{kl} = \begin{pmatrix} I^{kl}(1, \frac{1}{2}) & & & \\ & I^{kl}(\frac{1}{2}, 1) & & \\ & & I^{kl}(\frac{1}{2}, 0) & \\ & & & I^{kl}(0, \frac{1}{2}) \end{pmatrix} \tag{14}$$

We associate spinor matrices $A^{\lambda\dot{\mu}}$ with the tensor matrices a^k by

$$A^{\lambda\dot{\mu}} = a^m \sigma_m^{\ \lambda\dot{\mu}} \tag{15a}$$

Then

$$a^m = \tfrac{1}{2}\sigma^m_{\mu\lambda} A^{\lambda\dot{\mu}} \tag{15b}$$

Similarly we associate two symmetric spinor matrices $K^{\mu\nu}$ and $L^{\dot{\mu}\dot{\nu}}$ with the antisymmetric tensor I^{kl} by:

$$4K_\nu^{\ \mu} = -\, I_{mn}\, \sigma^{m\dot{\mu}\lambda} \sigma^{\ n}_{\lambda\nu} \tag{16a}$$

$$4L_{\mu}^{\ \dot{\lambda}} = I_{mn}\, \sigma^{\ m}_{\mu\nu} \sigma^{\dot{n}\nu\dot{\lambda}} \tag{16b}$$

Bhabha (1945) has shown that for a decomposition such as (13) one can write $A^{\lambda\dot{\mu}}$ as the direct products of certain known matrices:

$$\left.\begin{aligned} (k, l \mid A^{\beta\dot{\lambda}} \mid k + \tfrac{1}{2},\ l - \tfrac{1}{2}) &= cv^\beta (k + \tfrac{1}{2})\, u^{\dot{\lambda}}(l) \\ (k + \tfrac{1}{2}, l - \tfrac{1}{2} \mid A^{\beta\dot{\lambda}} \mid k, l) &= du^\beta (k + \tfrac{1}{2})\, v^{\dot{\lambda}}(l) \\ (k, l \mid A^{\beta\dot{\lambda}} \mid k + \tfrac{1}{2}, l + \tfrac{1}{2}) &= ev^\beta (k + \tfrac{1}{2})\, v^{\dot{\lambda}}(l + \tfrac{1}{2}) \\ (k + \tfrac{1}{2}, l + \tfrac{1}{2} \mid A^{\beta\dot{\lambda}} \mid k, l) &= fu^\beta (k + \tfrac{1}{2})\, u^{\dot{\lambda}}(l + \tfrac{1}{2}) \end{aligned}\right\} \tag{17}$$

all other components being zero. c, d, e, f are constants; $u^{\rho}(k)$ are the $(2k+1)\times 2k$ matrices and $v^{\rho}(k)$ are the $2k\times(2k+1)$ matrices introduced by Dirac [*cf.* eqns. (47) and (48) of Bhabha, 1945], which satisfy the following relations:

$$\left.\begin{aligned} -u_{\mu}(k+\tfrac{1}{2})\,v^{\mu}(k+\tfrac{1}{2}) &= v_{\mu}(k)\,u^{\mu}(k) = 2k+1\\ v_{\mu}(k)\,v^{\mu}(k+\tfrac{1}{2}) &= u_{\mu}(k+\tfrac{1}{2})\,u^{\mu}(k) = 0\\ -v^{\mu}(k+\tfrac{1}{2})\,u_{\nu}(k+\tfrac{1}{2}) &= \mathrm{K}_{\nu}{}^{\mu}(k) + (k+1)\,\delta_{\nu}{}^{\mu}\\ -u^{\mu}(k)\,v_{\nu}(k) &= \mathrm{K}_{\nu}{}^{\mu}(k) - k\,\delta_{\nu}{}^{\mu}, \end{aligned}\right\} \tag{18}$$

with similar relations for $u^{\dot{\mu}}(k)$, $v_{\nu}^{\dot{}}(k)$ in which $\mathrm{K}_{\nu}{}^{\mu}$ is replaced by $\mathrm{L}_{\dot{\nu}}{}^{\dot{\mu}}$.

In our case we have

$$\left.\begin{aligned} (1,\tfrac{1}{2}\mid \mathrm{A}^{\mu\dot{\lambda}}\mid \tfrac{1}{2},1) &= du^{\mu}(1)\,v^{\dot{\lambda}}(1)\\ (\tfrac{1}{2},1\mid \mathrm{A}^{\mu\dot{\lambda}}\mid 1,\tfrac{1}{2}) &= cv^{\mu}(1)\,u^{\dot{\lambda}}(1)\\ (1,\tfrac{1}{2}\mid \mathrm{A}^{\mu\dot{\lambda}}\mid \tfrac{1}{2},0) &= d'u^{\mu}(1)\,u^{\dot{\lambda}}(\tfrac{1}{2})\\ (\tfrac{1}{2},0\mid \mathrm{A}^{\mu\dot{\lambda}}\mid 1,\tfrac{1}{2}) &= c'v^{\mu}(1)\,v^{\dot{\lambda}}(\tfrac{1}{2})\\ (\tfrac{1}{2},1\mid \mathrm{A}^{\mu\dot{\lambda}}\mid 0,\tfrac{1}{2}) &= d''u^{\mu}(\tfrac{1}{2})\,u^{\dot{\lambda}}(1)\\ (0,\tfrac{1}{2}\mid \mathrm{A}^{\mu\dot{\lambda}}\mid \tfrac{1}{2},1) &= c''v^{\mu}(\tfrac{1}{2})\,v^{\dot{\lambda}}(1)\\ (\tfrac{1}{2},0\mid \mathrm{A}^{\mu\dot{\lambda}}\mid 0,\tfrac{1}{2}) &= d'''u^{\mu}(\tfrac{1}{2})\,v^{\dot{\lambda}}(\tfrac{1}{2})\\ (0,\tfrac{1}{2}\mid \mathrm{A}^{\mu\dot{\lambda}}\mid \tfrac{1}{2},0) &= c'''v^{\mu}(\tfrac{1}{2})\,u^{\dot{\lambda}}(\tfrac{1}{2}) \end{aligned}\right\} \tag{19}$$

By actual multiplication we have from (9)

$$a = \tfrac{3}{8}\,g_{kl}\,\alpha^{k}\,\alpha^{l} = \tfrac{3}{8}\,\alpha^{k}\,\alpha_{k} = \tfrac{3}{8}\,\{(\alpha^{0})^{2} - (\alpha^{1})^{2} - (\alpha^{2})^{2} - (\alpha^{3})^{2}\}$$

$$= \begin{pmatrix} \mathrm{I}_6 & \cdot & \cdot & \cdot\\ \cdot & \mathrm{I}_6 & \cdot & \cdot\\ \cdot & \cdot & \cdot & \cdot\\ \cdot & \cdot & \cdot & \cdot \end{pmatrix} \tag{20}$$

where I_6 is the 6×6 unit matrix. Also, from (15)

$$a = \tfrac{3}{8}\,\alpha^{k}\,\alpha_{k} = \tfrac{3}{16}\,\mathrm{A}_{\rho\dot{\mu}}\,\mathrm{A}^{\dot{\mu}\rho}$$

using (19) and (18) we have

$$\begin{aligned}(1, \tfrac{1}{2} \mid a \mid 1, \tfrac{1}{2}) &= \tfrac{3}{16}(1, \tfrac{1}{2} \mid \mathrm{A}_{\rho\dot{\mu}} \mid \tfrac{1}{2}, 1)(\tfrac{1}{2}, 1 \mid \mathrm{A}^{\rho\dot{\mu}} \mid 1, \tfrac{1}{2}) \\ &+ \tfrac{3}{16}(1, \tfrac{1}{2} \mid \mathrm{A}_{\rho\dot{\mu}} \mid \tfrac{1}{2}, 0)(\tfrac{1}{2}, 0 \mid \mathrm{A}^{\rho\dot{\mu}} \mid 1, \tfrac{1}{2}) \\ &= \tfrac{3}{16}\, du_\rho(1)\, v_{\dot{\mu}}(1) \cdot cv^\rho(1)\, u^{\dot{\mu}}(1) \\ &+ \tfrac{3}{16}\, d'u_\rho(1)\, u_{\dot{\mu}}(\tfrac{1}{2}) \cdot c'v^\rho(1)\, v^{\dot{\mu}}(\tfrac{1}{2}) \\ &= \tfrac{3}{16}(-6cd + 2c'd').\end{aligned}$$

With (20) this gives

$$-6cd + 2c'd' = \tfrac{16}{3}.$$

Similarly taking other components of a we arrive at

$$\begin{aligned} -6cd + 2c''d'' &= \tfrac{16}{3} \\ 6c''d'' - 2c'''d''' &= 0 \\ 6c'd' - 2c'''d''' &= 0 \\ dd'' &= -d'd''' \\ cd' &= -d''c''' \\ c'd &= -d'''c'' \\ cc'' &= -c'c''', \end{aligned}$$

whence

$$\begin{aligned} c = 1, d = -1, c' = -1, d' = \tfrac{1}{3} \\ c'' = 1, d'' = -\tfrac{1}{3}, c''' = 1, d''' = -1. \end{aligned}$$

In order to express I^{kl} in terms of α^k we try linear combinations of terms like

$$(\alpha^k \alpha^l - \alpha^l \alpha^k), (a\,\alpha^k \alpha^l - a\,\alpha^l \alpha^k), (a\,\alpha^k a\,\alpha^l - a\,\alpha^l a\,\alpha^k),$$

etc. [*cf.*, eqn. (3) above]. We calculate the different blocks of the two symmetric spinors which can be associated to each of the above terms by relations like (16), utilizing (19) and (18) and compare them with the corresponding blocks of $\mathrm{K}_\gamma{}^\mu$ and $\mathrm{L}_{\dot{\mu}}{}^{\dot{\nu}}$. In this way we obtain the result.

$$\begin{aligned} \mathrm{I}^{kl} = \tfrac{2}{5}(\alpha^k\alpha^l - \alpha^l\alpha^k) - \tfrac{3}{2}(\alpha^k\, a\,\alpha^l - \alpha^l\, a\,\alpha^k) \\ - \tfrac{39}{8}(a\,\alpha^k\alpha^l\, a - a\,\alpha^l\,\alpha^k\, a) + \\ + \tfrac{11}{2}(a\,\alpha^k\, a\,\alpha^l\, a - a\,\alpha^l\, a\alpha^k\, a). \end{aligned}$$

I am greatly indebted to Professor H. J. Bhabha who suggested the problem and guided the work.

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ON THE CHARACTERISTIC VIBRATIONS OF LINEAR LATTICES

By K. S. Viswanathan

(From the Raman Research Institute, Bangalore)

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Introduction

It is proposed in this paper to discuss the problem of the dynamical behaviour of a system which may be regarded as an one-dimensional analogue of a crystal, *viz.*, an extended chain of connected particles with a periodic structure, in other words, consisting of a great number of similar units each of which is made up of a finite number of particles with different masses held together by forces of interaction. To simplify the analysis, it is assumed that each particle interacts only with its immediate neighbours; otherwise, no restriction is laid upon the magnitude of the interacting forces.

The paper is divided into five parts. Parts I and II deal with the propagation of waves in a periodic linear lattice with p particles in each unit cell, and it is shown that the group velocities of the waves traversing the lattice vanish for $(2p-1)$ frequencies, which we call the characteristic frequencies of the lattice. In Parts III and IV, the spreading of an initial disturbance localised in a finite region of the lattice over its entire length is considered and an important result is established, *viz.*, that the resulting vibration of the particles of the lattice becomes a superposition of these $(2p-1)$ characteristic vibrations.[1] The application of the preceding results to crystal physics and the nature of the normal modes of vibration of periodic lattices are discussed in Part V.

I. Wave Propagation in Linear Lattices[2]

We shall consider a linear lattice of polyatomic molecules, consisting of p atoms in its unit cell. Each cell contains one period of the lattice and the masses of the particles in any cell are denoted by $m_1, m_2, \ldots . m_p$. We assume small displacements of the particles when a wave propagates along the lattice, but we restrict the interaction of the particles to their immediate neighbours alone. The force constant between the qth and the $(q+1)$th particles of any cell is represented by σ_q, σ_1 denoting the interaction constant between the last particle in any cell and its neighbour in the next cell. The notation adopted here is explained in Fig. 1, where the small circles indicate the equilibrium positions of the particles and the vertical lines the boundaries of any cell.

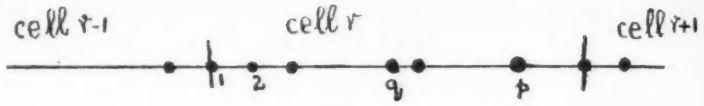

FIG. 1

If $x_{q,r}$ denotes the displacement of the qth particle in the rth cell about its equilibrium position, the equations of motion for the particles in the rth cell are given by

$$\begin{aligned}
-m_1\ddot{x}_{1,r} &= (\sigma_p + \sigma_1)\, x_{1,r} - \sigma_p x_{p,r-1} - \sigma_1 x_{2,r} \\
-m_q\ddot{x}_{q,r} &= (\sigma_{q-1} + \sigma_q)\, x_{q,r} - \sigma_{q-1} x_{q-1,r} - \sigma_q x_{q+1,r} \quad (q = 2, 3 \ldots p-1) \\
-m_p\ddot{x}_{p,r} &= (\sigma_{p-1} + \sigma_p)\, x_{p,r} - \sigma_{p-1} x_{p-1,r} - \sigma_p x_{1,r+1}
\end{aligned} \tag{1}$$

If we take the zero configuration for the potential energy as the energy of the lattice when all the particles are in their equilibrium positions, and assume that the displacements of the particles from their mean positions are due to an initial disturbance imparted to a finite region of the lattice, then the total energy of the lattice is a finite constant; in this case, the above equations can easily be obtained from a Lagrangian formulation. The expressions for the kinetic and potential energies of the lattice are given by

$$2\mathrm{T} = \sum_r \sum_q m_q \dot{x}_{q,r}^2 \tag{1a}$$

$$2\mathrm{V} = \sum_r \left[\sigma_p (x_{1,r} - x_{p,r-1})^2 + \sum_{q=1}^{p-1} \sigma_q (x_{q+1,r} - x_{q,r})^2 \right]$$

the summation extending over all the cells of the lattice. It can easily be seen that Lagrange's equations of motion for the particles of the rth cell of the lattice reduce to equations (1).

We shall assume wave solutions for equations (1) of the form

$$x_{q,r} = f_q e^{i(wt - r\theta)} \qquad (q = 1, 2, \ldots p), \tag{2}$$

where f and w are functions of the real variable θ.

Each of these p equations represents a wave propagating through particles of the same type in the lattice arrangement. The frequencies and wavelengths for a given disturbance must be equal, but the amplitudes of the waves are not necessarily equal; they may differ in phase as well as in magnitude. The amplitudes of the displacements of equivalent particles in successive cells are equal when a wave passes through them, but their phases change continuously.

Substituting the set of equations (2) in (1) we get

$$
\begin{aligned}
&a_1 f_1 - \sigma_1 f_2 - \sigma_p f_p e^{i\theta} = 0 \\
&-\sigma_{q-1} f_{q-1} + a_q f_q - \sigma_q f_{q+1} = 0 \quad (q = 2, 3, \ldots . p-1) \quad (3) \\
&-\sigma_p f_1 e^{-i\theta} - \sigma_{p-1} f_{p-1} + a_p f_p = 0
\end{aligned}
$$

where

$$a_q = (\sigma_{q-1} + \sigma_q - m_q w^2), \qquad (q = 2, 3, \ldots . p)$$

and

$$a_1 = (\sigma_p + \sigma_1 - m_1 w^2)$$

Eliminating the f's from the equations (3), we get

$$
\begin{vmatrix}
a_1 & -\sigma_1 & \cdot & \cdot & \cdot & & & -\sigma_p e^{i\theta} \\
-\sigma_1 & a_2 & -\sigma_2 & \cdot & & & & \\
\cdot & -\sigma_2 & a_3 & -\sigma_3 & \cdot & & & \cdot \\
\cdot & \cdot & \cdot & \cdot & & & & \cdot \\
 & & & & & & & \\
 & & & & & & & \\
\cdot & & & & & -\sigma_{p-2} & a_{p-1} & -\sigma_{p-1} \\
-\sigma_p e^{-i\theta} & & & & & & -\sigma_{p-1} & a_p
\end{vmatrix} = 0 \qquad (4)
$$

Expanding this determinant along the first row and column by Cauchy's method, we get

$$a_1 A_{11} - \sigma_1^2 |\, A_{11,22} | - \sigma_1 \sigma_p e^{-i\theta} |\, A_{11,2p} | - \sigma_1 \sigma_p e^{i\theta} |\, A_{11,p2} | - \sigma_p^2 |\, A_{11,pp} | = 0 \quad (5)$$

If we denote the (ij)th element of the above determinant by a_{ij} and the cofactor of a_{ij} by A_{ij}, then $-|\, A_{11,ij} \,|$ represents the cofactor of a_{i1} in $|\, A_{1j} \,|$. The notation is adopted from Aitken's *Determinants and Matrices*.[3]

It can easily be seen that $|\, A_{11,2p} \,| = |\, A_{11,p2} \,|$ and each is equal to $\sigma_2 \sigma_3 \ldots . \sigma_{p-1}$.

Hence (5) becomes

$$\Delta_p (w^2) - \sigma_p^2 \,|\, A_{11,pp}^{(w^2)} \,| = 2\sigma_1 \sigma_2 \ldots . \sigma_p \cos \theta \qquad (6)$$

where

$$
\Delta_p (w^2) = \begin{vmatrix}
a_1 & -\sigma_1 & \cdot & \cdot & & & \cdot \\
-\sigma_1 & a_2 & -\sigma_1 & \cdot & & & \\
\cdot & -\sigma_2 & a_3 & -\sigma_3 & & & \\
 & & & & & & \\
 & & & & & & \\
\cdot & & & & -\sigma_{p-2} & a_{p-1} & -\sigma_{p-1} \\
\cdot & & & & \cdot & -\sigma_{p-1} & a_p
\end{vmatrix}
$$

$|A_{11,pp}|$ can be obtained by suppressing the first and the last rows and columns of the above determinant.

From the difference equations satisfied by the continuants, it can easily be proved that

$$\Delta_p(0) = \sigma_1\sigma_2.\ldots.\sigma_p\left(2 + \sum_{r=1}^{p-1}\frac{\sigma_p}{\sigma_r}\right) \tag{7}$$

and

$$|A_{11,pp}^{(0)}| = \sigma_1\sigma_2.\ldots.\sigma_{p-1}\sum_{r=1}^{p-1}\frac{1}{\sigma_r}. \tag{8}$$

Hence the term independent of w in (6) is equal to $2\sigma_1\sigma_2..\sigma_p(1-\cos\theta)$.

Equation (6) can be expressed as a polynomial in w^2 and we can rewrite (6) as

$$\phi(w^2) = s_0w^{2p} + s_1w^{2p-2} + \cdot + s_{p-t}w^{2t} + \cdot + s_p(1-\cos\theta) = 0 \tag{9}$$

The coefficients $s_0, s_1, \ldots. s_p$ are expressed below as symmetric functions in the masses and force constants of the lattice.

$$s_0 = (-1)^p m_1m_2.\ldots.m_p$$

$$s_1 = (-1)^{p-1}m_1m_2.\ldots.m_p\left(\sum_{r=1}^{p}\frac{\sigma_{r-1}+\sigma_r}{m_r}\right), \text{ where } \sigma_0 = \sigma_p.$$

$$s_{p-t} = (-1)^t\,\sigma_1\sigma_2.\ldots.\sigma_p\,\Sigma\, m_{i_1}m_{i_2}.\ldots.m_{i_t}\,(A-B). \tag{10}$$

where

$$A = \left(\frac{1}{\sigma_p}+\frac{1}{\sigma_1}+..+\frac{1}{\sigma_{i_1-1}}\right)\left(\frac{1}{\sigma_{i_1}}+\frac{1}{\sigma_{i_1+1}}+\cdot+\frac{1}{\sigma_{i_2}}\right).\ldots.$$
$$\left(\frac{1}{\sigma_{i_t}}+\frac{1}{\sigma_{i_t+1}}+\cdot+\frac{1}{\sigma_p}\right)$$

and

$$B = \left(\frac{1}{\sigma_1}+\frac{1}{\sigma_2}+\cdot+\frac{1}{\sigma_{i_1-1}}\right)\left(\frac{1}{\sigma_{i_1}}+\frac{1}{\sigma_{i_1+1}}+..+\frac{1}{\sigma_{i_2}}\right)\cdots$$
$$\left(\frac{1}{\sigma_{i_t}}+\frac{1}{\sigma_{i_t+1}}+\cdot+\frac{1}{\sigma_{p-1}}\right).$$

The summation above extends over all the different t combinations of the symbols $i_1, i_2, \ldots. i_p$ which represent the first p natural numbers in some order or other. We assume without loss of generality that the i's in any term of the summation are arranged in order of increasing magnitude. The two different sums involving A and B in (10) represent the coefficient of w^{2t} in $\Delta_p(w^2)$ and $\sigma_p^2\,|A_{11,pp}|$ respectively; clearly $(A-B)$ is positive and B vanishes when $i_1 = 1$ or $i_t = p$.

$$s_{p-1} = -\sigma_1\sigma_2.\ldots.\sigma_p(m_1+m_2+\cdot+m_p)\left(\frac{1}{\sigma_1}+\frac{1}{\sigma_2}+\ldots.+\frac{1}{\sigma_p}\right)$$
$$s_p = 2\sigma_1, \sigma_2.\ldots.\sigma_p.$$

s_q and s_{q-1} being always of the opposite signs, it follows from Descarte's rule of signs that equation (9) cannot have any negative roots for w^2 and hence all its roots are real and positive. $\frac{\partial \phi}{\partial w^2}$ is a polynomial of degree $(p-1)$ in w^2 with constant coefficients and hence all the roots of $\frac{\partial \phi}{\partial w^2} = 0$ are independent of θ. It follows that (9) cannot have any multiple root which is a function of θ. In this paper, we consider only the case of non-degenerate vibrations in which all the roots of (9) are different for all values of θ in $(0, 2\pi)$. Since (9) is an equation of degree p in w^2, for each value of θ we get p values for w^2 which are the roots of (9).

From (3) and (9) we can easily see that f and w are periodic functions of θ with period 2π and hence the values of θ outside the range $(-\pi, \pi)$ are mere repetitions of those inside the closed interval $-\pi \leqslant \theta \leqslant \pi$ for $x_{q,r}$ in (2). Therefore, we write

$$-\frac{1}{2d} \leqslant \frac{1}{\lambda} \leqslant \frac{1}{2d}, \text{ where } \frac{1}{\lambda} = \frac{\theta}{2\pi d} \tag{11}$$

$\therefore |\lambda| \geqslant 2d$ and hence the shortest wavelength equals twice the lattice spacing.

II. Group Velocity of the Waves

Differentiating (9) with respect to θ, we arrive at the following expression for the group velocity of the waves traversing the lattice

$$\frac{dv}{d\left(\frac{1}{\lambda}\right)} = \mathrm{U}(\theta) = \frac{-s_p d \sin\theta}{2w\left(ps_0 w^{2p-2} + (p-1)s_1 w^{2p-4} + \ldots + s_{p-1}\right)}. \tag{12}$$

When $\theta = \pi$, $\frac{dv}{d\left(\frac{1}{\lambda}\right)}$ vanishes and thus for each of the p frequencies corresponding to this value of θ, the group velocity of the waves vanishes. When however $\theta = 0$, one of the roots of (9) becomes zero and the expression (12) tends to a definite limit $d\sqrt{\frac{-s_p}{s_{p-1}}}$ corresponding to this zero frequency. For the remaining $(p-1)$ roots of (9) which are non-zero, the expression (12) is equal to zero. *Thus, for a lattice with* p *particles in its unit cell, there are* (2p $-$ 1) *characteristic frequencies for which the group velocities of the waves are zero.*

The group velocity is the velocity with which the maximum amplitude of a train of waves of a given frequency travels and for an observer moving with this velocity in the direction of propagation of the waves, the disturbance will turn into an approximately simple harmonic wave-train of an assigned wave-length λ. The fact that the group velocity of the waves corresponding

to the $(2p-1)$ characteristic frequencies vanishes is highly significant and implies that wave clusters corresponding to these characteristic frequencies do not move at all while individual waves may spread along the lattice with their wave velocities. Hence if a finite region of the lattice suffers an initial disturbance, all wave clusters other than those that correspond to the limiting frequencies would have spread along both sides of the lattice so that after a certain time, the motion of the particles near the domain of initial disturbance will be predominantly influenced by wave-trains with zero group velocity. It follows that the state of movements of these particles is one of a stationary vibration, consisting of a superposition of the $(2p-1)$ characteristic vibrations of the lattice—a result that is rigorously proved in Section III.

III. EFFECT OF AN INITIAL DISTURBANCE

In this Section, we discuss the spreading of an initial disturbance in the form of small displacements of a group of particles in any cell into those regions which were previously undisturbed. Due to the interaction of the particles with their neighbours, the energy concentrated in a limited region of the lattice is progressively transferred to the entire length of the lattice and thus all the particles are set in agitation and execute small oscillations about their mean positions. The general expressions for the displacements of the particles from their mean positions can be obtained by superposing wave solutions of the type (2) for all values of θ lying in one period of w, *i.e.*, within the closed interval $(0, 2\pi)$. Hence, if we denote the roots of (9) by $w_1, w_2 \ldots . w_p$; $-w_1, -w_2, \ldots . -w_p$ and the corresponding values of f_q by $f_{q,1}$; $f_{q,2}$; $\ldots . f_{q,p}$; $f_{q,p+1}$; $\ldots . f_{q,2p}$ respectively, the general expressions are given by

$$x_{q,r} = \frac{1}{4\pi} \sum_{s=1}^{p} \int_0^{2\pi} [f_{q,s}(\theta)\, e^{iw_s t} + f_{q,s+p}(\theta)\, e^{-iw_s t}]\, e^{-ir\theta} d\theta$$

$$(q = 1, 2, \ldots . p) \qquad (13)$$

Let us now suppose that initially all the particles in the cell with index zero are displaced by small amounts and the velocities and displacements of all other particles are zero.

$$(i.e.)\ x_{q,r}(0) = \alpha_q \delta_{r0} \text{ and } \dot{x}_{q,r}(0) = 0 \qquad (14)$$

for all q and r.

Then from (13) we get

$$x_{q,r}(0) = \frac{1}{4\pi} \sum_{s=1}^{p} \int_0^{2\pi} (f_{q,s} + f_{q,s+p})\, e^{-ir\theta}\, d\theta. \qquad (15)$$

Let us now expand $\sum_{s=1}^{p}(f_{q,s}+f_{q,s+p})$ as a Fourier series in the form $\sum_{s=0}^{p}(f_{q,s}+f_{q,s+p})=\sum_{-\infty}^{+\infty}A_k\,e^{ik\theta}$ so that $A_k=\frac{1}{2\pi}\int_0^{2\pi}\sum_{s=1}^{p}(f_{q,s}+f_{q,s+p})\,e^{-ik\theta}\,d\theta$. Then from (13) and (14) we get

$$a_q=\frac{1}{4\pi}\int_0^{2\pi}(f_{q,s}+f_{q,s+p})\,d\theta$$

$$0=\frac{1}{4\pi}\int_0^{2\pi}(f_{q,s}+f_{q,s+p})\,e^{-ir\theta}\,d\theta \text{ for all } r\neq 0.$$

Since $\frac{1}{2\pi}\int_0^{2\pi}e^{i(k-r)\theta}\,d\theta=\delta_{kr}$, we get

$$\sum_{s=1}^{p}(f_{q,s}+f_{q,s+p})=2a_q\ (q=1,2,\ldots.p) \tag{16}$$

Similarly, from (14) we get

$$0=\frac{1}{4\pi}\sum_{s=1}^{p}\int_0^{2\pi}w_s(f_{q,s}-f_{q,s+p})e^{-ir\theta}\,d\theta \text{ for all } r.$$

$$\therefore\ \sum_{s=1}^{p}w_s(f_{q,s}-f_{q,s+p})=0\ (q=1,2,\ldots.p) \tag{17}$$

Now, from the set of equations (3), the ratios of the quantities $f_1, f_2 \ldots f_p$ can be uniquely determined. Let us suppose that when $w=w_s$, the ratios are given by

$$f_{1,s}:f_{2,s}:\ldots.:f_{p,s}=g_1(w_s^2):g_2(w_s^2):\quad :g_p(w_s^2).$$

Also, since the equations (3) are unaffected by writing $-w$ for w, we have

$$f_{1,s+p}:f_{2,s+p}:\ldots.:f_{p,s+p}=g_1(w_s^2):g_2(w_s^2):\ldots.:g_p(w_s^2).$$

We shall write $f_{q,s}=\lambda_s g_q(w_s^2)$ and $f_{q,s+p}=\lambda_{s+p}g_q(w_s^2)$ (18)

The g's are known from equations (3) and the λ's are the unknown quantities. By substituting (18) in (16) and (17) we get $2p$ equations in the λ's which enable us to determine them in terms of the g's and α's. Thus the equations (3) together with the initial conditions are sufficient to determine the f's. To obtain the actual values of the f's as functions of the frequencies of the waves, the following procedure may be adopted. From the initial conditions (14) and the set of equations (1), the initial values of the higher derivatives of the displacements of the particles can be determined and hence from the initial values of the derivatives of order up to $(2p-1)$ of the displacements of the particles, we get the following $2p$ linearly independent equations

$$\sum_{s=1}^{p} w_s^{2r} (f_{q,s} + f_{q,s+p}) = h_{q,r} \; (r = 0, 1, \ldots . p-1) \tag{19}$$

$$\sum_{s=1}^{p} w_s^{2r+1} (f_{q,s} - f_{q,s+p}) = 0 \quad (r = 0, 1, \ldots . p-1). \tag{20}$$

where $h = h(m, \alpha, \sigma, \theta)$. For example, $h_{q,o} = 2\alpha_q$, etc. Since by assumption the roots of (9) are all different, the square matrix of the coefficients of $(f_{q,s} - f_{q,s+p})$ in (20) is non-singular and hence it follows that

$$f_{q,s} = f_{q,s+p} \; (q, s = 1, 2, \ldots . p) \tag{21}$$

The equations (13) can now be written as

$$x_{q,r} = \frac{1}{4\pi} \sum_{s=1}^{p} \int_{0}^{2\pi} f_{q,s} \, (e^{iw_s t} + e^{-iw_s t}) \, e^{-ir\theta} \, d\theta$$

$$= \frac{1}{4\pi} \sum_{s=1}^{p} \int_{-\beta}^{2\pi-\beta} f_{q,s} \, (e^{iw_s t} + e^{-iw_s t}) \, e^{-ir\theta} \, d\theta \quad (q = 1, 2, \ldots . p) \tag{22}$$

where $O < \beta < \pi$ (since f and w are periodic functions of θ).

We shall find the asymptotic value of the above integral for large values of t by employing Kelvin's method of stationary phase.[4] When $w_s t$ is large compared to r, $\cos w_s t$ is a rapidly oscillating function and hence the maximum contribution of the above integral arises from those points at which w_s is stationary (*i.e.*) at the points where $\frac{dw_s}{d\theta} = 0$. $\therefore \quad \theta = 0$ or π.

Now the asymptotic value of the integral[4] $I = \int_a^b f(x) \, e^{iw(x)t} \, dx$ for large values of t is given by

$$I \sim \sum_{x_0} \frac{\sqrt{2\pi} \, f(x_0) \, e^{i\left(w(x_0)t \pm \frac{\pi}{4}\right)}}{| \, w''(x_0) \, t \, |^{\frac{1}{2}}}$$

where the positive or negative sign in the exponent is to be taken according as $w''(x_0)$ is positive or negative and the summation extends over all the points in the interval (a, b) which are solutions of the equation $\frac{dw}{dx} = 0$.

Applying this result to (22), we find that the asymptotic value of $x_{q,r}$ for large values of t is given by

$$x_{q,r} = \left(\frac{1}{2\pi t}\right)^{\frac{1}{2}} \sum_{s=2}^{p} \frac{f_{q,s}(0)}{| \, w_s''(0) \, |^{\frac{1}{2}}} \cos\left(v_s t \pm \frac{\pi}{4}\right)$$

$$+ (-1)^r \left(\frac{1}{2\pi t}\right)^{\frac{1}{2}} \sum_{s=1}^{p} \frac{f_{q,s}(\pi)}{| \, w_s''(\pi) \, |^{\frac{1}{2}}} \cos\left(v_{s+p} t \pm \frac{\pi}{4}\right),$$

$$(q = 1, 2, \ldots . p) \tag{23}$$

wherethe positive or negative sign in the cosine terms is to be taken according as $w_s''(\theta_0)$ $(\theta_0=0, \pi)$ is positive or negative. v_s and v_{s+p} are the values of $w_s(\theta)$ when $\theta = 0$ and π. $f(0)$ and $f(\pi)$ are real and $v_1 = 0$. *Hence, asymptotically*

(1) *the state of vibration of the particles tends to a superposition of the* $(2p-1)$ *characteristic vibrations of the lattice and*

(2) *the amplitudes of vibrations of the particles vary inversely as the square root of the time elapsed.*

IV. Particular Cases

As a particular case of the above general theory, we shall consider the vibrations of a monatomic linear lattice which was first studied by Hamilton in connection with his researches on the theory of the dispersion of light.[5] The equation of motion for the rth particle is given by $m\ddot{x}_r = \sigma(x_{r-1} + x_{r+1} - 2x_r)$, where m is the mass of any particle and σ is a force constant.

If we assume wave solutions for the above equations of the form

$$x_r = f(\theta)\, e^{i(wt - r\theta)} \tag{24}$$

we can easily see that w is given by the roots of the equation

$$mw^2 = 4\sigma \sin^2 \theta/2. \tag{25}$$

If the initial conditions are $x_r(0) = a\delta_{r0}$

$$\text{and } \dot{x}_r(0) = 0 \tag{26}$$

for all r, then the general expressions (22) for the displacements of the particles about their equilibrium positions reduce to

$$\begin{aligned} x_r &= \frac{a}{4\pi}\int_0^{2\pi} (e^{ivt} + e^{-ivt})\, e^{-ir\theta}\, d\theta \\ &= \frac{a}{\pi}\int_0^{\pi} \cos(vt \sin\theta) \cos 2r\theta d\theta \\ &= aJ_{2r}(vt), \end{aligned} \tag{27}$$

where $v = \sqrt{4\sigma/m}$—we arrive at the same result obtained by Hamilton in a different way.

Hence when vt is large compared to r, the asymptotic value of (27) becomes

$$x_r = \left(\frac{2}{\pi vt}\right)^{\frac{1}{2}} (-1)^r \cos\left(vt - \frac{\pi}{4}\right) \tag{28}$$

showing that the motion is periodic with a frequency that is precisely the characteristic frequency of the lattice.

It is interesting to consider the way in which the nth particle begins its motion. The Bessel function attains its maximum value when its argument is slightly greater than its order so that the maximum amplitude of this particle is attained only after a time given by the inequality $vt > 2n$. Also since $J_{2n}(z)$ approaches zero as z^{2n} and the first value of z for which $J_{2n}(z)$ vanishes lies between $\sqrt{2n(2n+2)}$ and $\sqrt{2(2n+1)(2n+3)}$, we can easily see that the larger n is, the slower is the beginning of the motion and a longer time does this particle take to reach its maximum in one direction. Finally, when vt is large compared to n so that the asymptotic approximation for the Bessel function can be applied to (28), all the masses within the belt $\pm nd$ and those in the neighbourhood of the nth particle vibrate with the limiting frequency of the lattice, consecutive particles always oscillating with opposite phases.

The case $p = 2$ corresponds to the vibrations of a linear lattice of diatomic molecules which was recently discussed by Nagendra Nath and S. K. Roy.[6,7] By evaluating the values of the f's as functions of the frequencies of the waves, we can easily see that (23) reduces to the expressions obtained by these authors by using the method of steepest descents.

V. SOME GENERAL REMARKS

The dependence of the amplitudes of the particles on time is instructive and indicates that the vibrations decay slowly, the law of decrease being $t^{-\frac{1}{2}}$. This is due to the fact that the initial energy is progressively transferred to the neighbouring cells and the amplitude of any particle is proportional to the square root of its vibrational energy. The damping of the vibrations suggests the possibility of restricting our discussion to a finite but long linear lattice, with its ends far from the region of initial disturbance. In such a case, the outgoing cluster of waves would have almost died out before it reaches the end and gets reflected, and hence the boundary exerts practically an insignificant influence on the subsequent vibrations of the particles of the lattice. Again for all observations confined within the time-limit T which is the time taken by the fastest group to reach the end, the above analysis holds good rigorously and T can be made sufficiently large by taking the length of the lattice great enough.

Restricting ourselves to the region in which the disturbance has settled into a stationary mode of oscillation, the asymptotic form (23) suggests a striking similarity of the vibrations of the particles with the normal modes

of vibrations of polyatomic molecules characterised by a common frequency and phase for the vibrations of all the atoms of the molecule. The displacements of the particles of the lattice from their equilibrium positions arise due to the transmission of the initial energy by waves of all possible wavelengths and amplitudes to them, but the asymptotic state of their movements is built up of a superposition of $(2p-1)$ normal modes of vibration which differ entirely in their behaviour from a wave-motion involving a continuous change in the phases of particles. The $(2p-1)$ characteristic modes of vibration fall into two classes, one consisting of $(p-1)$ modes in which equivalent particles in successive cells vibrate with the same phase and amplitude at any instant, while in the other p modes due to the dependence of the amplitudes on the factor $(-1)^r$, equivalent particles in successive cells vibrate with opposite phases. Thus there is a complete agreement of these results with the general theory for three-dimensional lattices proposed by Sir C. V. Raman[1] that a crystal with p atoms in its unit cell has $(24p-3)$ normal modes of vibration of which $21p$ modes belong to a set in which vibration occurs with alternate layers moving with opposite phases while in the remaining $(3p-3)$ modes, equivalent particles in consecutive cells vibrate with the same amplitudes and phases.

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Summary

The nature of wave propagation in a linear lattice consisting of p particles in its unit cell has been studied and it is shown that the group velocity of the waves corresponding to each of the $(2p-1)$ characteristic frequencies of the lattice is identically equal to zero. It has been further proved that the state of movements of the particles resulting from an initial disturbance localised in a finite region of the lattice tends asymptotically to a superposition of the $(2p-1)$ characteristic vibrations of the lattice. In $(p-1)$ modes of these vibrations, equivalent particles in successive cells vibrate with the same phases and amplitudes, while in the remaining p normal modes, vibration occurs with equivalent particles moving alternately with opposite phases. These results form an one-dimensional analogue of the general theory of vibrations of crystal lattices formulated by Sir C. V. Raman and are generalisations of the results corresponding to the cases $p=1$ and $p=2$ which were first obtained respectively by Hamilton and by Nagendra Nath and S. K. Roy. In view of the decay of the amplitudes of vibrations of the particles with time, these results hold good for a finite lattice

also, provided its length is sufficiently large and the domain of initial disturbance is far from its ends.

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